Recurrent flow analysis in spatiotemporally chaotic 2-dimensional Kolmogorov flow

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Motivated by recent success in the dynamical systems approach to transitional flow, we study the efficiency and effectiveness of extracting simple invariant sets (recurrent flows) directly from chaotic/turbulent flows and the potential of these sets for providing predictions of certain statistics of the flow. Two-dimensional Kolmogorov flow (the 2D Navier-Stokes equations with a sinusoidal body force) is studied both over a square \([0, 2\pi]^2\) torus and a rectangular torus extended in the forcing direction. In the former case, an order of magnitude more recurrent flows are found than previously (Chandler & Kerswell 2013) and shown to give improved predictions for the dissipation and energy pdfs of the chaos via periodic orbit theory. Over the extended torus at low forcing amplitudes, some extracted states mimick the statistics of the spatially-localised chaos present surprisingly well recalling the striking finding of Kawahara & Kida (2001) in low-Reynolds-number plane Couette flow.

At higher forcing amplitudes, however, success is limited highlighting the increased dimensionality of the chaos and the need for larger data sets. Algorithmic developments to improve the extraction procedure are discussed.

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I. INTRODUCTION

Recent years have seen an increasing trend towards a dynamical systems approach to the study of at least chaotic if not turbulent flows. While this approach has already seen considerable success in the study of transition to turbulence [1–4], it is very much still in its infancy when applied to fully turbulent flows [4–6]. Here, the basis of the approach is the idea of a turbulent flow being represented by a point in phase space tracing out a trajectory in time which fleetingly but repeatedly visits the neighbourhoods of simple invariant sets (exact solutions of the governing questions) embedded in the phase space [7]. During such a visit the flow trajectory is attracted along the (typically very high dimensional) stable manifold of the simple invariant set before being expelled along its (typically much lower-dimensional) unstable manifold, the flow transiently takes on the properties of the simple invariant set. Given enough of these invariant sets, the hope is then that an appropriately weighted sum of all their properties could be used to predict those of the turbulent flow. This approach has proved fruitful for very low-dimensional hyperbolic systems [8–11] where periodic orbit theory (POT) is used to weight the various invariant set contributions. However, the application to very high dimensional turbulent flows is less clear and hugely challenging (see [6] for a discussion).

The situation is not without hope, though, as the breakthrough computation in 2001 of Kawahara and Kida [12] indicated. These authors managed to isolate a single periodic orbit embedded in the turbulent attractor in a 15,422 degree-of-freedom simulation of small-box plane Couette flow at low Reynolds number. The velocity statistics of this one orbit were found to be remarkably similar to those of the turbulent state itself (see their figure 3). Encouraged by this success, subsequent work has concentrated on trying to extract further simple invariant sets from direct numerical simulations - a process hereafter referred to as recurrent flow analysis - to improve this correspondence [6, 13–18]. However progress has been slow due the many challenges surrounding this approach starting with how best to identify simple invariant sets - hereafter recurrent flows - from turbulent simulations (and subsequently converge them to machine accuracy), followed by how best to weight the contribution of each recurrent flow in a prediction, to finally deciding how many such flows are needed to achieve a required prediction accuracy. So far, the furthest this approach has been pushed for the Navier-Stokes equations is in 2-dimensional Kolmogorov flow [6] where 50 recurrent flows were found at a relatively low level of forcing and used to postdict an array of key statistics of the (weakly) turbulent flow. Various weighting strategies were tested alongside periodic orbit theory with the conclusion that not enough recurrent flows had been extracted to see the theory outperform even a simple-minded ‘democratic’ approach of equal weighting. Furthermore, attempts to repeat the procedure at a higher level of forcing failed to produce enough recurrent flows to even attempt a prediction. A number of reasons for this failure were discussed, but undoubtedly the most likely reason was that the extent of turbulent flow data used to identify recurrent flows needed to be much larger. One objective here is to revisit this calculation by generating and then processing such an extended data set.

The second objective is to make a first attempt to study an extended system where spatiotemporal behaviour is possible. Here, a further, more fundamental challenge emerges: how far can one push this approach when the apparent correlation length of the flow is smaller than the domain size? Formally, nothing has changed in the sense that global recurrent flows still exist to the full dynamical system produced by the Navier-Stokes equations applied over the whole domain. Informally, however, the fact that the correlation length is smaller than the domain implies that the flow never fully ‘approaches’ such ‘global’ states in phase space. Practically, this would seem to make the identification of near-recurrences (from the turbulent flow data) good enough to converge to exact recurrent flows considerably more difficult. A possible way to circumvent this could be to focus on sub-domains where coherence is identified to isolate perhaps localised recurrent flow states but this raises fresh issues such as what boundary conditions to impose on the sub-domain. To start exploring these important issues, we treat - i.e. apply recurrent flow analysis to - the spatiotemporal flows recently discovered in [19] by extending the domain of 2-dimensional Kolmogorov flow in the forcing direction. Here, a series of states exhibiting spatially-localised chaos were found which present an ideal opportunity to broach these issues. Finally, since the method to carry out this recurrent flow analysis is still relatively new and unsophisticated, we also take the opportunity to discuss issues surrounding the technique and developments undertaken to improve difficulties.

The plan of the paper is as follows. The formulation of 2D Kolmogorov flow studied here is described in section II and exactly follows the set up described in [6, 19]. The results are presented in two sections: section III describes the square torus and $Re = 60$ calculations and section IV details the computations carried out on the various chaotic states present in the extended domain case. A final section V discusses all the results and indicates future directions.
II. FORMULATION

Kolmogorov flow is the name given to body-forced incompressible viscous flow over a doubly periodic domain where the forcing is steady and monochromatic [20] so that the governing equations are

\[
\frac{\partial \mathbf{u}^*}{\partial t^*} + \mathbf{u}^* \cdot \nabla \mathbf{u}^* + \frac{1}{\rho} \nabla^* p^* = \nu \Delta^* \mathbf{u}^* + \chi \sin(2\pi ny^*/L_y) \hat{x},
\]

\[
\nabla^* \cdot \mathbf{u}^* = 0
\]

where \( \mathbf{u} = u\hat{x} + v\hat{y} = (u, v) \) is the two-dimensional velocity field, \( n \) is the forcing wavenumber, \( \chi \) the forcing amplitude, \( \nu \) kinematic viscosity, \( p \) pressure and \( \rho \) is the density of the fluid defined over the doubly periodic domain \( (x, y) \in [0, L_x] \times [0, L_y] \). The system is naturally non-dimensionalised with lengthscale \( L_y/2\pi \) and timescale \( \sqrt{L_y/2\pi \chi} \) to give

\[
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = \frac{1}{Re} \Delta \mathbf{u} + \sin n y \hat{x},
\]

\[
\nabla \cdot \mathbf{u} = 0
\]

where we define the Reynolds number

\[
Re := \sqrt{\chi} \left( \frac{L_y}{2\pi} \right)^{3/2}
\]

and take \( n = 4 \) throughout as in [6] [19]. The equations are solved over the torus \([0, 2\pi/\alpha] \times [0, 2\pi]\) where \( \alpha = L_y/L_x \) defines the aspect ratio of the domain with \( \alpha = 1 \) in [11] and \( \alpha = \frac{1}{2} \) in [14]. For computational efficiency and accuracy [3] is formulated so that vorticity \( \omega := \nabla \times \mathbf{u} \) is the prognostic variable and the vorticity equation

\[
\frac{\partial \omega}{\partial t} + \mathbf{u} \cdot \nabla \omega = \frac{1}{Re} \Delta \omega - n \cos ny
\]

is solved numerically using the GPU timestepping code presented in [19]. Vorticity is discretised via a Fourier-Fourier spectral expansion with resolution \( N_x \times N_y \) and dealiased by the two-thirds rule;

\[
\omega(x, y, t) = \sum_{k_x=0}^{N_x/3-1} \sum_{k_y=-N_y/3}^{N_y/3-1} \Omega_{k_x,k_y}(t) e^{i(\alpha k_x x + k_y y)}.
\]

A Crank-Nicolson timestepping scheme is used for the viscous terms and Heun’s method for the nonlinear and forcing terms. Typical numerical resolutions used were 128 Fourier modes per \( 2\pi \) so \((N_x, N_y) = (128, 128)\) for \( \alpha = 1 \) and \((N_x, N_y) = (512, 128)\) for \( \alpha = 1/4 \). Typical time steps were \( dt = 0.05 \) at \( Re = 20 \) and \( 0.001 \) at \( Re = 120 \) with \( 2 \times 10^6 \) time steps \( (dt = 0.05, T = 10^5) \) of the \( 512 \times 128 \) grid for \( \alpha = 1/4 \) and \( Re = 20 \) taking 63 minutes on a 512-core NVIDIA Tesla M2090 GPU. The system has the following symmetries:

\[
S: [u, v](x, y) \rightarrow [-u, v](-x, y + \frac{\pi}{n}),
\]

\[
R: [u, v](x, y) \rightarrow [-u, -v](-x, -y),
\]

\[
T_l: [u, v](x, y) \rightarrow [-u, v](x + l, y), \quad \text{for } 0 \leq l \leq \frac{2\pi}{\alpha}
\]

where \( S \) represents the discrete shift-and-reflect symmetry relative to the forcing, \( R \) rotation through \( \pi \) and \( T_l \) is the group of continuous translations in \( x \). In order to discuss various features of the flows considered we define the total energy, dissipation and energy input:

\[
E(t) := \frac{1}{2} \langle |\mathbf{u}|^2 \rangle_A, \quad D(t) := \frac{1}{Re} \langle |\nabla \mathbf{u}|^2 \rangle_A, \quad I(t) := \langle u \sin ny \rangle_A
\]

as diagnostic quantities where the area average is defined as

\[
\langle \cdots \rangle_A := \frac{\alpha}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi/\alpha} \cdots \, dr dy.
\]
Mean flow and rms (root mean square) fluctuation velocities are defined by
\[
U(y) := \langle u \cdot \hat{x} \rangle_{t,x}, \quad u_{rms}^2(t) := \langle (u - U)^2 \rangle_A, \quad v_{rms}^2(t) := \langle v^2 \rangle_A, \tag{11}
\]
(initial conditions are set so the mean of \(v\) is zero and therefore will be zero for all time). The variation of the rms quantities only with \(y\) is brought out by the quantities
\[
u_{rms}^2(y) := \langle (u - U)^2 \rangle_{t,x}, \quad v_{rms}^2(y) := \langle v^2 \rangle_{t,x}, \tag{12}
\]
where
\[\langle \cdots \rangle_t := \lim_{T \to \infty} \frac{1}{T} \int_0^T \cdots \, dt, \quad \langle \cdots \rangle_x := \frac{\alpha}{2\pi} \int_0^{2\pi/\alpha} \cdots \, dx.\]

The base state, or laminar profile, is given by
\[
u_{lam} := \frac{Re}{n^2} \sin ny \hat{x} \tag{13}
\]
with its energy \(E_{lam} := Re^2/4n^2\) and dissipation, \(D_{lam} := Re/2n^2\) used for normalisation purposes.

The purpose of this work is to discuss the extraction of recurrent flows from simulation data of a chaotic/turbulent 2D Kolmogorov flow. To do this we follow the methodology described in section 3.2 of [6]. Briefly, ‘near recurrences’ are defined as episodes in the DNS where
\[
\mathcal{T}_s \mathcal{S}^{2m} \omega(x, y, t + T) := \omega(x + s, y + \frac{1}{2} \pi m, t + T) = \omega(x, y, t) \tag{14}
\]
‘approximately’ holds for some choice of the continuous shift \(0 \leq s < 2\pi\), the discrete shift \(m \in \{0, 1, 2, \ldots, n - 1\}\) and \(T > 0\) over \(0 \leq x, y < 2\pi\). This expression reflects the presence of the system symmetries \(\mathcal{T}_s\) and \(\mathcal{S}^2\) but not \(\mathcal{R}\) and \(\mathcal{S}\) which was a choice made in [6] for reasons of expediency: recurrent flows of period \(T\) with these suppressed symmetries are captured by (14) as recurrent flows with period \(2T\). In (14), periodic orbits correspond to \(s = m = 0\) and some period \(T > 0\), travelling waves (TWs) to \(m = 0\) and \(s = cT\) with \(T > 0\) free where \(c\) is the phase speed, equilibria have \(s = m = 0\) and \(T\) free and relative periodic orbits have one or both of \(s\) and \(m\) not equal to zero with period \(T > 0\). Once a near-recurrent event has been found, a Newton-GMRES-hookstep algorithm was employed to try to converge an exactly recurrent flow (at least to double precision accuracy). The algorithm used is as described in [6] albeit with the underlying time-stepping part of the process carried out on a GPU card to make the procedure faster.

III. RESULTS: SQUARE TORUS (\(\alpha = 1\)) AT \(Re = 60\)

In this first section of results, we revisit the square torus chaos that was the focus of [6]. There it was found that at higher Reynolds numbers (\(Re > 40\)) longer integrations were necessary to assemble a large enough set of recurrent flows to enable a meaningful analysis using POT. Focussing on \(Re = 60\), an extended direct numerical simulation (DNS) was conducted to \(T = 5 \times 10^6\) which is 50 times longer than each of the 3 runs analysed in [6]. Near-recurrences of the flow were recorded during the simulation to be used as initial guesses in a Newton-GMRES-hookstep rooting-finding algorithm afterwards.

A. Recurrence extraction and convergence

To expedite the extraction of guesses for recurrent flows, the recurrence criterion of [6] was modified slightly. Instead of defining a close recurrence based on the normalised difference of the full state vector, we included only the 8 largest modes in either direction;
\[
R(t, T) := \min_{0 \leq s \leq 2\pi/\alpha} \min_{m \in \{0, 1, 2, \ldots, n - 1\}} \left\| \sum_{k_x=0}^{8} \sum_{k_y=-8}^{8} \Omega_{k_x,k_y}(t)e^{i(k_x \alpha s - 2k_y m \pi/\alpha)} - \sum_{k_x=0}^{8} \sum_{k_y=-8}^{8} \Omega_{k_x,k_y}(t) \right\|^2 < R_{thres} \tag{15}
\]
FIG. 1. Distribution of recurrence guesses from the $Re = 60$, $\alpha = 1$ DNS calculation with $T = 5 \times 10^6$ and $R_{thres} = 0.3$. Left plot shows a histogram of total recurrences determined in $\Delta T = 1.0$ windows. Right plot shows the distribution of residuals for the guesses with $R_{thres} = 0.3$ on log scale.

In comparisons with the ‘full’ recurrence check ($N_x = N_y = 128$ so $\max k_x = \max k_y = 42$), this reduced criterion was found to capture almost every near-recurrence but crucially gave a huge computational saving: there was a 14 times speed up compared to the full state vector criterion (see Table III in Appendix A and the discussion there for other recurrence criteria).

Setting the residual threshold $R_{thres} = 0.3$, the DNS calculation yielded 11,934 guesses for when the flow appeared to repeat; figure 1 shows the distribution of these guesses over period, $T$, and residual, $R$. The exponential increase in the number of guesses with increasing $R$ is probably a cumulative effect since recurrences discovered with a small residual are also likely to be visited ‘less closely’, i.e. with a larger residual, at about the same time. The variation with period $T$ is marked by a large skew toward low periods, i.e. $T < 5.0$, which reflect close visits to unstable steady and travelling wave states. For larger periods ($T > 20$), there is little variation in the numbers of guesses found. This is somewhat counterintuitive since it should become less probable that the trajectory shadows a recurrent flow the longer its period if the leading Lyapunov exponent is largely period-independent.

From these guesses we converged 81 unique recurrent flows: see Table IV in appendix B and figure 2. At low periods, there was a large repetition of the converged solutions already found in [6] ($E_1, T_1, T_3, T_4, R_7, R_8$ and symmetry group permutations thereof) and so only about a third of the guesses with $T < 5.0$ were processed. Likewise for $T > 60.0$, no recurrences with $R < 0.25$ converged so we focussed computational resources on periods $0.5 < T < 60.0$ and skipped recurrences with $R > 0.25$ (this filtering still meant attempts were made to converge 5,120 of the total 11,934 guesses).

Figure 3 shows the success rate of converging near-recurrence guesses into exactly recurrent flows as a function of the starting residual. As is expected, there is a negative correlation but it is weak: for example the chances of converging a guess settle to about 10% for $R \gtrsim 0.2$.

B. Cycle expansions

We now examine how the extended set of relative periodic orbits (RPO: now totalling 86 with the 5 found in [6]) can be used to predict properties of 2D turbulent Kolmogorov flow at $Re = 60$. The basic idea is to develop an appropriately weighted expansion across the set of relative periodic orbits as follows

$$\Gamma^{N}_{\text{prediction}} := \frac{\sum_{i=1}^{N} w_i \Gamma_i}{\sum_{i=1}^{N} w_i}$$

where the property $\Gamma$ could be the mean dissipation rate, the mean profile or a pdf, $\Gamma_i$ is the property value and $w_i$ the weight for the $i$th RPO, and $N$ is a finite but large number (to be discussed below). In periodic orbit theory, the weights cannot be simply expressed but instead emerge from a recursive construction in which the RPOs (‘prime cycles’) are arranged in progressively longer sequences (‘pseudo-cycles’) which each contribute until a cut-off is applied [11]. As in
FIG. 2. The stabilities $\Lambda_i$ (see the definition in (17)) of the 86 periodic and relatively periodic recurrent flows at $Re = 60$ (blue filled circles with the original 5 found in [6] having an extra circle). The black dashed line indicates $\Lambda_{\text{max}}(82)$, the fifth largest value, used for the stability cut-off. The periods $T$ of the recurrent flows (red filled squares) are also shown to indicate that there is a weak positive correlation with stability.

FIG. 3. Figure showing the convergence success rate for the guesses at $Re = 60$ with a given starting residual (see figure 1). Red circles indicate where the total guesses are less than 10, blue diamonds have total guesses less than 100 (and more than 10) and black squares have over 100 guesses. Note increased variability at small $R$ where the number of guesses is small and the trend toward a fixed success rate when the sample size increases with larger $R$.

[6], the dynamical-zeta-function periodic orbit averaging formula is used since this only needs information about the (typically much smaller number of) unstable Floquet multipliers rather than the whole spectrum. If $\Lambda_k^{(i)} := e^{\Re(\lambda_k^{(i)})T_i}$ is the modulus of the $k$th Floquet multiplier of the linearised (Jacobian) operator around the $i$th recurrent flow of period $T_i$ ($\lambda_k^{(i)}$ the complex growth rate), then the weight associated with the $i$th recurrent flow depends on

$$\Lambda_i := \prod_{k, \Lambda_k^{(i)} > 1} \Lambda_k^{(i)} = \exp(\sum_{k \in K_i} \Re(\lambda_k^{(i)})T_i).$$

(17)
(see e.g. 21, 22, §20 of 11) where $K_i$ is the set of $k$ such that $\Re (\Lambda_k) > 0$. For bounded flows (no trajectories escape - see §20.4.1 11), the zeta-function averaging formula takes the (relatively) simple form

$$\Gamma_{\text{prediction}} := \frac{\langle \Gamma \rangle}{\langle T \rangle}$$

(18)

where

$$\langle \Gamma \rangle := \sum_{\pi} (-1)^{k+1} \frac{\sum_{i=1}^{k} T_{p_i} \Gamma_{p_i}}{\Lambda_{p_1} \Lambda_{p_2} \cdots \Lambda_{p_k}}$$

(19)

and

$$\langle T \rangle := \sum_{\pi} (-1)^{k+1} \frac{\sum_{i=1}^{k} T_{p_i}}{\Lambda_{p_1} \Lambda_{p_2} \cdots \Lambda_{p_k}}$$

$$= \sum_{i=1}^{k} T_i - \sum_{i=1}^{k} \sum_{j=i+1}^{k} \Lambda_i \Lambda_j + \sum_{i=1}^{k} \sum_{j=i+1}^{k} \sum_{k=j+1}^{k} \frac{T_i + T_j + T_k}{\Lambda_i \Lambda_j \Lambda_k} - \cdots$$

(20)

(see §20.4.1 11). Here the subscript $p_i$ refers to the $p_i$ th prime cycle (taken to be all the recurrent flows identified), $\Gamma_{p_i}$ is the temporal average of the quantity $\Gamma$ over this cycle and $\sum_{\pi}^{'}$ represents a sum over all $(k = 1, 2, 3, \ldots)$ non-repeating, ordered combinations of prime cycles making up a pseudo-cycle (e.g. $\pi = (p_1, p_2, p_3, \ldots, p_k)$ represents a pseudo-cycle of prime cycles $p_1$ to $p_k$ concatenated to create a total period of $\sum_{i=1}^{k} T_{p_i}$). Very roughly, the geometrical meaning of a pseudo-cycle is that it is a sequence of shorter periodic orbits that shadow a longer periodic orbit along the segments $p_1, p_2, \ldots, p_k$ with the relative minus signs ensuring shadowing cancellations.

As in 6, a cut-off strategy is adopted based upon stability 23, 24, §20.6 11 in which only pseudo-cycles with

$$\Lambda_{p_1} \Lambda_{p_2} \cdots \Lambda_{p_k} \leq \Lambda_{\text{max}}$$

(21)

are included: this indirectly sets $N$. Usually $\Lambda_{\text{max}}$ is set as $\max_i \Lambda_i$ across all the prime cycles found. However, figure 2 which shows how $\Lambda_i$ increases across all the (suitably reordered) 86 relative periodic flows known at $Re = 60$, indicates that the 4 most unstable cycles are outliers. As a result we took $\Lambda_{\text{max}} = 2.98 \times 10^7$ which corresponds to $\Lambda_i$ for the fifth most unstable cycle (shown as a dashed black line in figure 2) for the calculations shown. There is no discernable difference, however, to the results based upon $\Lambda_{\text{max}} = \max_i \Lambda_i$.

As a benchmark against which to assess the performance of periodic orbit theory, we also considered a control protocol consisting of a ‘democratic’ equal weighting,

$$w_i := 1$$

(22)

across all the relative periodic orbits (note in 3, this was protocol 3 and also included a very small number of equilibria and travelling waves also found). The key measures we look to predict are pdfs of the total kinetic energy $E(t)$ and the total dissipation rate $D(t)$ together with the profiles of the mean flow $\bar{u}(y)$ and root-mean-square-profiles of the fluctuation fields, $u_{rms}(y)$ and $v_{rms}(y)$.

The pdfs of $E(t)/E_{\text{lam}}$ and $D(t)/D_{\text{lam}}$ are shown in figure 4 along with the predictions using periodic orbit theory (expression 18, magenta line with squares) and the control protocol (dashed black line). The control prediction is very good across the maximum of the kinetic energy pdf but fails not surprisingly to capture the lower shoulders ($E(t)/E_{\text{lam}} > 0.36$ and $E(t)/E_{\text{lam}} < 0.26$). The POT prediction is noticeably worse and dominated by two peaks which indicate the presence of two different groups of RPOs with separated energy levels. To confirm this interpretation, the POT prediction was recalculated excluding the first 4 least unstable RPOs (since they look like a separate group stability-wise in figure 2) and the first 11 least unstable RPOs (where again there is a discernable change in the stability of the RPOs) with the results shown in figure 5. This clearly shows that the first 4 least unstable RPOs are responsible for the first peak in the pdf centred on $E/E_{\text{lam}} \approx 0.29$. Also shown but difficult to distinguish from the full POT prediction is a prediction based only on the prime cycles (black solid line). This indicates that including the pseudo-cycles has very little effect on the scale of this plot.

The control prediction for the normalised dissipation rate pdf $D(t)/D_{\text{lam}}$ is very good near the maximum but again fails to capture the broad lower shoulder in the pdf at higher dissipation rates. Similarly the POT prediction is not so effective, overestimating the pdf peak and failing to capture the lower dissipation behaviour of the dissipation rate as well as the higher-dissipation shoulder. Interestingly, excluding the first group of least unstable RPOs from the POT prediction improves matters at least at low dissipation rates: see figure 5. Again, there is little effect in excluding
FIG. 4. The probability density functions for $E(t)/E_{lam}$ (left) and $D(t)/D_{lam}$ (right) from DNS (blue thick line) and predictions using periodic orbit theory (magenta, thick line with squares) and the control (black thick dashed) at $Re = 60$. 60 bins were used to calculate the pdfs for the recurrent flows and 100 bins for the DNS due to its greater range. These choices gave the best balance of resolution with the data available.

pseudo-cycles (see the overlapping solid black line - just prime cycles included - and the magenta line with squares - the full POT prediction in figure 5).

Given the poor representation of higher-dissipation DNS episodes, an effort was made to revisit the data to particularly focus on these. The original 11,934 guesses were filtered down to just 68 guesses which had an average dissipation larger than the long time average of the DNS calculation. These represent infrequent, high-dissipation ‘bursting’ events first noticed in [6] and now recognised in [19] as intense interactions of spatially localised ‘kink’ and ‘anti-kink’ regions (see §IV below). Not surprisingly, these 68 guesses also had longer periods (predominantly $T > 40$) and none could be converged. A revised recurrent flow check was also tried in which large $k = |k|$ wavenumbers were preferentially weighted to favour small scale/high dissipation flows;

$$R(t, T) := \min_{0 \leq s \leq 2\pi/\alpha} \min_{m \in 0, 1, \ldots, n-1} \frac{\sum_{k_x=0}^{32} \sum_{k_y=-32}^{32} k |\Omega_{k_xk_y}(t) e^{i(k_x\alpha s - 2k_y m\pi/n)} - \Omega_{k_xk_y}(t-T)|^2}{\sum_{k_x=0}^{32} \sum_{k_y=-32}^{32} k |\Omega_{k_xk_y}(t)|^2} < R_{thres}$$

(note that the sums now need to retain more of the larger wavenumbers). Taking a test run of $T = 2 \times 10^4$ and a threshold of $R_{thres} = 0.5$ produced 30 recurrent guesses with high dissipation although none, again, could be converged.

Turning to the flow profiles, it was remarked in [6] that a run of $10^5$ time units at $Re = 60$ was not long enough to see a (long-time-averaged) mean flow sharing all the symmetries of the system. This assumed, by default, that the turbulent attractor is unique and correspondingly that the mean should achieve this state of full symmetry if the simulation was long enough. However, the reduced-symmetry mean state found in [6] could have been one of many co-existing turbulent attractors selected by the initial conditions. It was therefore interesting to simulate the flow for much longer - here $50 \times$ longer - to check the uniqueness of the attractor. Figure 6 (left) reproduces the 3 different means generated in [6] using 3 different initial conditions each integrated over $1 \times 10^5$ time units which clearly shows that they individually are not invariant under $\pi/2$ shifts in $y$ let alone under $S$. Figure 6 (right) shows the mean (plotted as blue dots) from the new $5 \times 10^6$ data set. The red solid line (upon which the mean blue dots basically sit) is the symmetrised version of the mean defined as

$$U^{SR}(y) := \frac{1}{2^n} \sum_{m=0}^{2n-1} S^{-m} U^R(S^m y) \quad \text{with} \quad U^R := \frac{1}{2} [U(y) + R^{-1}U(Ry)]$$
FIG. 5. The probability density functions for $E(t)/E_{lam}$ (left) and $D(t)/D_{lam}$ (right) from DNS (blue thick line) and the predictions from POT (magenta, solid line with squares), POT theory excluding pseudocycles (black solid line), POT with the first 4 least unstable UPOs removed (red dashed line) and POT with the first 11 least unstable UPOs removed (dash-dot green line).

FIG. 6. Left: DNS mean flows from runs $e$, $f$ and $g$ (see Table 1 of [6]) at $Re = 60$ showing a lack of convergence even after $10^5$ time units (this is a reproduction of figure 22(b) of [6]). Right: DNS mean flow from $5 \times 10^6$ time units showing the expected symmetrisation: the DNS mean flow plotted across $[0, 2\pi]$ using blue dots essentially coincides with the symmetrised DNS shown as a solid red line.

(recall $n = 4$) which satisfies all the symmetries of the flow (this process picks out the following Fourier coefficients

$$U^{SR}(y) := \sum_{m=0} a_m \sin(4(2m + 1)y)$$

from the complete Fourier series of the mean flow $U(y)$. The mean flow is essentially fully symmetric indicating that the attractor is unique and that $5 \times 10^6$ should be sufficiently long to generate worthwhile statistics. A similar symmetrisation was also carried out for the root-mean-square profiles of the fluctuation velocities to generate $u_{rms}^{SR}$ and $v_{rms}^{SR}$. Such symmetrised profiles need only be plotted over $y \in [0, \pi/4]$ which is done in figure 7 along with the
FIG. 7. Left: The symmetrised mean flow $U_{SR}(y)$ (DNS - solid blue), the POT prediction (magenta line with open squares) and control prediction (black dashed line) at $Re = 60$. Right: symmetrised $u_{rms}^{SR}(y)$ (DNS - blue solid line with filled dots, POT prediction - magenta line with filled squares and control prediction - black dashed line with diamonds) and $v_{rms}(y)$ (DNS - blue solid line, POT prediction - magenta line with open squares and control prediction - dashed black line) over $[0, \pi/4]$.

POT and control predictions. Both the POT and control predictions perform well (with POT doing best) for $U_{SR}$ and $v_{rms}$ (the three lines to the far right of figure 7) but are noticeably poor for $u_{rms}^{SR}$ which has a value near 1 across the domain whereas the predictions never get above 0.4 anywhere. The poor match in $u_{rms}^{SR}$ could be related to the lack of representation of high dissipation bursts in the recurrent flows extracted. One such orbit was identified at $Re = 40$ in [6] (named $R50$) and shown in figures 11 and 12 there. The large $D$ excursion at approximately $t = 8$ of this orbit can be seen to exhibit strong horizontal velocity, suggestive that these events will contribute to the $u_{rms}$ profile heavily.

Some progress has been made from [6] - we have identified an order of magnitude more recurrent flows and the POT predictions are much improved (e.g. contrast figures 4 and 26a from [6]). However, periodic orbit theory is still not outperforming a simple minded ‘democratic’ averaging of the RPO properties despite the nearly two orders of magnitude of RPOs isolated. The lumpiness of the kinetic energy pdf prediction in particular highlights how a small number of weakly unstable RPOs can dominate affairs due to the extreme sensitivity of the weighting of an RPO to its stability (recall the Floquet multipliers are exponentiated). Periodic orbit theory is clearly vulnerable to wide disparities in stability across small sets of identified RPOs which typically don’t reflect the true distribution across the turbulent attractor. This situation should, of course, be ameliorated by finding even more RPOs - perhaps $O(1000)$ would emerge by increasing the simulation time by another factor of 50 - but it also suggests some better feel for phase space as a whole is needed to improve matters. For example, are some of the longer period prime cycles actually pseudo-cycles? (and therefore being counted incorrectly.) Are all of the converged RPOs actually in the turbulent attractor or just coincidentally converged from the DNS due to the vagaries of the Newton algorithm in high dimensions? And where is the best place to look to possibly ‘fill in’ missing prime cycles (those of short period and weak instability or those exhibiting the high $D$ bursting events) whose contribution is being overlooked?

IV. RESULTS: LONG DOMAIN ($\alpha = 1/4$)

We now turn our attention to applying recurrent flow analysis to the rich spatiotemporal behaviour found in [19] when 2D Kolmogorov flow is solved over a domain extended in the forcing direction. The flow response mimicks the forcing at low forcing amplitudes but, as in the square torus, beyond a critical value develops a linear instability. This instability selects the longest wavelength allowed with the flow displaying Cahn-Hilliard-type (coarsening) dynamics for slightly higher $Re$ (see [19] and references herein). The unique attractor in this regime very quickly (as $Re$ increases), develops two equal-length regions where the flow is 1-dimensional joined together by localised 2D adjustment regions - a ‘kink’ and an ‘antikink’; see figure 8. Following this state to higher $Re$, the kink and antikink pair suffer a sequence of instabilities so that by $Re = 40$, they are locally chaotic although the 1D states which they connect remain steady.
FIG. 8. Vorticity field, $\omega(x,y)$ at $Re = 25$ for the steady solution branch which emerges from the initial bifurcation in the $\alpha = 1/4$ domain (colour extrema are $\omega = -5$ black to $\omega = 5$ white and 5 evenly spaced contours in $-4 \leq \omega \leq 4$). Two 1-dimensional regions are joined together by a 'kink' (where the vorticity is a maximum i.e. to the side in the image) and an 'antikink' (where the vorticity is most negative i.e. in the middle here).

This chaos steadily intensifies as $Re$ increases to 120 and presents a good target for recurrent flow analysis. However, we start the discussion at lower $Re$ by focussing on another state, $P_1$, unearthed by [19] which exists in the window $11 \lesssim Re \lesssim 25$ where the flow possesses several attractors. The $P_1$ orbit is composed of a stationary kink-antikink pair flanking an inner region where two oppositely signed vorticity patches (resembling a kink-antikink pair in close proximity) interact to form an intertwined oscillatory behaviour; see figure 9 for ($x,y$) snapshots which resemble the flow. This inner region undergoes a period doubling cascade into chaos as $Re$ increases leaving the flanking kink and antikink pair still stationary. A boundary crisis at $Re = 24.1$ then converts this attractor into a (localised) chaotic repellor.

A. $P_1$ at $Re = 24$: chaotic attractor

At $Re = 24$, the $P_1$ orbit is a spatially localised chaotic attractor. Two DNS runs of duration $T = 10^5$ were generated and the reduced recurrence criterion [15] used to extract nearly recurrent flows. A threshold of $R_{thres} = 0.3$ yielded 89 guesses from which 2 unique periodic orbits were converged (3 convergences in total). Lowering the threshold to $R_{thres} = 0.2$ surprisingly yielded an order of magnitude more guesses, 935, from which another 2 periodic orbits were converged (23 convergences total). Table I outlines the characteristics and convergence frequencies of these 4 recurrent solutions (no steady states were found). Figure 9 shows snapshots and space-time projections for two of the flows; the short period ($T = 17.036$) flow is observed to exhibit a single internal oscillation, where the longer orbit ($T = 87.451$) has 5 such oscillations.

| $Re$  | $T$   | $s$   | $\sum_{Re(\lambda_i) > 0} Re(\lambda_i)$ | $freq. \ 1$ | $freq. \ 2$ |
|-------|-------|-------|------------------------------------------|-------------|-------------|
| 24    | 17.036| 4.5E-4| 0.0624                                   | 2           | 1           |
| 24    | 87.451| -1.9E-3| 0.0199                                   | 1           | 2           | 10          |
| 24    | 87.258| -7.5E-4| 0.0231                                   | 2           | 0           | 10          |
| 24    | 87.634| -2.9E-4| 0.0147                                   | 2           | 0           | 2           |
| 24.5  | 18.405| 9.0E-4| 0.2398                                   | 6           | 1           | 0           |
| 24.5  | 84.985| -1.3E-3| 0.0265                                   | 2           | 1           | 13          |
| 24.5  | 16.986| 3.9E-4| 0.0807                                   | 3           | 0           | 1           |

TABLE I. Converged solutions from the $Re = 24$ $P_1$-chaotic attractor and $Re = 24.5$ $P_1$-chaotic repellor. Columns freq. 1 and 2 indicate the number of times the recurrent flow was discovered from the calculation with $R_{thres} = 0.3$ and then $R_{thres} = 0.2$ respectively.

The apparently counterintuitive inverse correlation between the threshold level and the number of guesses found is actually due to the combination of two effects. The first is the fact that the recurrent flows at $Re = 24$ are only weakly unstable so that the flow spends a comparatively long time in their vicinity potentially appearing as multiple 'visits' in one episode. The second is the necessarily finite history window (chosen to be $[t-100,t]$) carried along by the recurrence checking algorithm which is usually long enough compared to the periods of the extracted flow. When $R$ dips below $R_{thres}$ indicating a nearly recurrent event, the algorithm waits for $R$ to next exceed $R_{thres}$ before searching across the retained history to store the velocity field at the smallest $R$. If there are a sequence of visits to an orbit such that $R$ repeatedly dips below and above $R_{thres}$, multiple guesses will be stored. If $R_{thres}$ is too high only the last visit will be stored when only one visit fits into last 100 time units: see figure 10 for an example of this.
This issue arises for weakly unstable recurrent flows of long period as found here at $Re = 24$.

Figure 11 shows the probability density function for the $P1$ chaos at $Re = 24$ over the energy dissipation $D$ and the difference between energy input and output, $I - D$, normalised by the laminar dissipation (in the coordinates $(D,I - D)$ the pdf is centred on the horizontal $I - D = 0$ rather than the usual diagonal $I = D$ in the $(I,D)$ plane). The four recurrent flows are also plotted and all look fairly similar. The fact that the majority of recurrent episodes found in the DNS had periods near to these orbits (figure 16) suggests that periodic orbit theory may work well. Using the cycle expansions of section III B, it was found that these few orbits reconstruct the flow statistics impressively (see figures 12 and 13; note that the mean profiles are not symmetrised and the control of democratic weighting does almost as well). In fact, since each of the longer orbits spans the DNS pdf well in figure 11, the second recurrent flow with $T = 87.451$ was chosen from Table 1 to compare its mean and rms velocities with those of the DNS: see figure 14. The profiles match remarkably well and recalls the earlier striking success of [12] which appeared to demonstrate that a single embedded recurrent flow was able to replicate the mean and rms velocity profiles of small-box turbulent plane Couette flow.
(I – D)/D_{lam} versus D/D_{lam} for the converged orbits from the P1-chaos at Re = 24. Grey shading shows the DNS pdf, the orbit with T = 17.036 is red and the longer orbits with periods ≈ 87 are drawn in green, blue and magenta.

The probability density functions for $E(t)/E_{lam}$ (left) and $D(t)/D_{lam}$ (right) from DNS (blue thick line) and the predictions from POT (magenta, solid line with squares) and control (black dashed line). Re = 24 P1 chaos and UPOs as in table I.

**B. P1 at Re = 24.5 chaotic transient**

After a boundary crisis at Re ≈ 24.1, the P1 chaotic attractor becomes a chaotic saddle which was studied at Re = 24.5 using recurrent flow analysis. The lifetime of the transient chaos here is $T ≈ 4.1E4$ and thus still relatively long despite apparently being close to the crisis. Setting $R_{thres} = 0.3$ yields 122 guesses from which only two recurrent flows were converged. Lowering the threshold to 0.2 gives 1842 recurrences from which two orbits were converged; one new and the other a repeat of one found at $R_{thres} = 0.3$ (converged solutions are listed in table I and shown...
FIG. 13. Left: The unsymmetrised mean flow $U(y)$ (DNS - solid blue), the POT prediction (magenta line with open squares) and control prediction (black dashed line) for the P1-chaos at $Re = 24$. Middle: unsymmetrised $u_{rms}(y)$ (DNS - blue solid line with filled dots, POT prediction - magenta line with filled squares and control prediction - black dashed line with diamonds). Right: $v_{rms}(y)$ (DNS - blue solid line, POT prediction - magenta line with open squares and control prediction - dashed black line) over $[0, 2\pi]$.

FIG. 14. Mean and r.m.s. velocities for the DNS (solid blue lines) and the recurrent flow with period $T = 87.451$ (green stars) with $Re = 24$. Left: The mean flow $U(y)$. Middle: $u_{rms}(y)$. Right: $v_{rms}(y)$ over $[0, 2\pi]$.

in figure 15. As with the attracting chaos of the previous section, there are only a few distinct periods within the set of recurrent guesses extracted from the DNS (figure 16). However, this time, the three orbits found have distinct characteristics. The $T = 18.405$ orbit, when viewed in the $(D, I - D)$ plane (figure 17) is visually more compact and does not span the attractor in the manner of the rest of the unstable flows discovered at $Re = 24$ or $Re = 24.5$. Branch continuing the orbits found at $Re = 24.5$ down to $Re = 24$ revealed that the shorter period orbit, $T = 16.986$ at $Re = 24.5$ is connected to the $T = 17.036$ orbit at $Re = 24$ but no other connections were found. The large period orbit, $T = 84.985$, at $Re = 24.5$ appears in these figures similar to the longer orbits of the sustained chaos at $Re = 24$. However, in this case the mean profiles (figure 18) do not match the DNS profiles. Figure 15 shows the space-time projection for the three orbits.
FIG. 15. Vorticity in an \((x,t)\) plane for \(y = 21\pi/32\) for the converged orbits from the P1-chaos at \(Re = 24.5\). Left shows the orbit with \(T = 18.405\) and right that with \(T = 84.985\). Colour extrema are \(\omega = -5\) black, \(\omega = 5\) white.

FIG. 16. Distribution of guesses with period for \(R_{\text{thres}} = 0.2\) and 0.3 for \(Re = 24\) (left) and \(Re = 24.5\) (right). Notice the distinct recurrent periods found, as opposed to the broader band recurrences at \(Re = 60\), with \(\alpha = 1\).

C. \(P1\) at \(Re = 30\) chaotic transient

At \(Re = 30\) the chaotic saddle has a much shorter mean lifetime and therefore a suite of 6 DNS were performed with a randomly perturbed (1% with randomised phase) initial condition in each case in order to build up a sufficiently long data sequence for recurrent flow analysis. Across the 6 calculations, lifetimes ranged from \(\approx 500\) time units up to 4500 time units. The threshold \(R_{\text{thres}} = 0.3\) yielded 218 recurrence guesses across the concatenated data set. Of these, 7 (time-dependent) recurrent flows were converged, each only once, as detailed in Table II. Figure 19 shows these flows and the probability density function for the chaotic repellor over the \((D/D_{\text{lam}},(I - D)/D_{\text{lam}})\) plane. The coverage of the pdf by the recurrent flows identified is much more limited than at lower \(Re\) and, not surprisingly, the ability of these recurrent flows to replicate the transient chaos is similarly reduced: see figure 20. However, figure 21 shows that the velocity predictions are better with the mean profile reproduced best (note the abscissa scales in figure 21).

D. \(Re = 40, 70\) & 120 kink-antikink chaos

The general trend from the above calculations is that while recurrent flows can still be extracted as \(Re\) increases, their predictive power (at least in the numbers found here) reduces. This, of course, is consistent with the usual
FIG. 17. $I - D$ versus $D$ for the converged orbits from the P1-chaos at $Re = 24.5$. Grey colours show the DNS p.d.f., cyan shows the orbit with $T = 18.405$, yellow that with $T = 84.985$ and red the $T = 16.98$ orbit as in figure [11].

FIG. 18. Mean and r.m.s. velocities for the DNS (solid blue lines) and the recurrent flow with period $T = 84.985$ (Red stars) at $Re = 24.5$. Left: The unsymmetrised mean flow $U(y)$. Middle: unsymmetrised $u_{rms}(y)$. Right: unsymmetrised $v_{rms}(y)$ over $[0, \pi]$. Increasing dimension of the chaos and presumably with the increasing number of simple invariant sets embedded in the chaos. In this section we consider yet higher $Re$ where the kink-antikink solutions, which are connected to the initial bifurcation point in Kolmogorov flow, become chaotic.

At $Re = 40$ with $R_{thres} = 0.3$, we extracted 200 guesses from a $T = 10^5$ long DNS data set and converge 7 unique steady states (out of 81 convergences), all of which fall on the known solution branches shown in figure 9 of [19]. A test investigation at $Re = 70$ found similar results using a smaller temporal integration for reasons of expediency (higher $Re$ requires a smaller timestep): from $T = 10^4$ with $R_{thres} = 0.3$ we found 263 guesses which is an order of magnitude more guesses in this more disordered regime from an order of magnitude shorter data set. From these guesses, those with $R < 0.1$ (54 guesses) were used to converge 2 distinct steady states (9 convergences) which again
TABLE II. Converged solutions from $Re = 30$ P1-chaotic repellor. DNS column indicates from which of the randomised initial conditions the unstable orbit was converged.

| $T$    | $s$  | $\sum \lambda$ | $N_\lambda$ | DNS |
|--------|------|-----------------|-------------|-----|
| 13.67  | 2.3E-3 | 0.216           | 7           | 1   |
| 17.24  | 8.6E-3 | 0.252           | 4           | 1   |
| 12.23  | -7.0E-3| 0.359           | 7           | 2   |
| 12.11  | -4.6E-3| 0.134           | 5           | 2   |
| 12.06  | -7.4E-3| 0.0848          | 4           | 2   |
| 13.32  | 1.1E-3 | 0.212           | 6           | 3   |
| 13.07  | 4.2E-4 | 0.202           | 4           | 4   |

FIG. 19. $I - D$ versus $D$ for the converged orbits from the P1-transient chaos at $Re = 30$. Grey colours show the DNS p.d.f. with statistics accumulated over the 6 calculations.

lie on known solution branches (figure 9 of [19]).

Some effort was also made at $Re = 120$: using a long $T = 10^5$ data set and $R_{thres} = 0.3$ gave 2984 guesses. In contrast with the $Re = 60$, $\alpha = 1$ calculations of section [11] these were unevenly distributed in period. Figure [22] shows that the majority of recurrences found have a period close to 11 and the rest are distributed around multiples of this value. This indicates that there is a dominant recurrent flow (or set of similar flows) which is expected to have a small number of unstable directions and is therefore visited frequently in the chaotic attractor. For this reason, and due to the higher computational burden at this Reynolds number ($dt = 0.002$), Newton-GMRES-hookstep efforts were concentrated on guesses with $T \approx 11$ but with no success: of 209 such guesses attempted none converged. Several attempts were also made for higher periods (e.g. $T \approx 22$, 33 etc.) without success.

Given the spatial localisation of the chaos in the kink-antikink solutions, one idea to improve the situation was to focus in on either the kink or antikink chaos when extracting recurrent flow guesses. This idea arose because, by $Re = 120$, the chaotic kink and antikink look effectively uncorrelated (except for the global constraint that the total vorticity is time-invariant). To check this, figure [22] shows the two-point correlation

$$C(x - x_{max}; x_{max}, y_0) := \int_0^T \hat{\omega}(x_{max}, y_0, t)\hat{\omega}(x, y_0, t)dt$$

(where $\hat{\omega}$ denotes the fluctuating part of the vorticity, $x_{max}$ denotes the $x$ location of peak vorticity - the kink - and the choice $y_0 = \pi$ was made arbitrarily) normalised by the autocorrelation $C(0; x_{max}, y_0)$ for various time intervals.
FIG. 20. The probability density functions for $E(t)/E_{lam}$ (left) and $D(t)/D_{lam}$ (right) from DNS at $Re = 30$ of the $P1$-transient chaos (blue thick line) and the predictions from POT (magenta, solid line with squares) and the control (black dashed line).

FIG. 21. Left: The mean flow $U(y)$ (DNS - solid blue line), the POT prediction (magenta line with open squares) and control prediction (black dashed line) at $Re = 30$. Middle: unsymmetrised $u_{rms}(y)$ (DNS - blue solid line, POT prediction - magenta line with filled squares and control prediction - black line with diamonds). Right: $v_{rms}(y)$ (DNS - blue solid line, POT prediction - magenta line with filled squares and control prediction - black line) over $[0, \pi/4]$.

The shrinking of the correlation near $x = -12$ (the antikink) with increasing $T$ indicates that the kink and antikink regions are uncorrelated. Armed with this, a revised recurrent flow check was devised which only focussed on a subset (containing the kink) of the full domain. This entailed working with the physical vorticity field $\omega$ in a region of width $15/16 \pi$ (60 collocation points) centred on the supremum of $\omega$ across the full $y$ range so that the residual function became

$$R(t, T) := \min_{m \in 0, 1, 2, n - 1} \frac{1}{i_{max} + 30} \sum_{i_x = i_{max} - 30}^{i_{max} + 30} \sum_{i_y = 0}^{N_y} \left| \omega(i_x \frac{8\pi}{N_x}, i_y \frac{2\pi}{N_y}, t) - \omega(i_x \frac{8\pi}{N_x}, i_y \frac{2\pi}{N_y}, t - T) \right|^2$$

$$< R_{\text{thres}}$$

(26)
where $i_x$ and $i_y$ are the collocation points (respecting periodicity at the boundaries) in the $x$ and $y$ directions respectively and $i_{\text{max}}$ is the $x$ index of the supremum of $\omega$. Since there was little drift of the chaotic attractor in $x$ (across the timescales of the DNS simulation), the shift $s$ was assumed zero but allowed to vary from this value in the Newton-GMRES-hookstep stage. Taking an integration length of $T = 10^4$ and a threshold $R_{\text{thres}} = 0.2$ yielded over 200 such guesses, all of which again failed to converge.

In both choices of residual function, (15) and (26), almost identical behaviour of the Newton-GMRES-hookstep algorithm was found. Typically the residual saturated at values significantly lower ($10^{-3}, 10^{-8}$) than the starting guess, but above the convergence criterion. This is suggestive that a limitation may exist at the Newton-GMRES stage rather than that the proximity of the individual guesses are poor.

V. DISCUSSION

In this paper we have applied recurrent flow analysis to 2D Kolmogorov flow over a square and rectangular torus. In the former case, a much longer data set (than previously [6]) has been generated in order to find more recurrent flows and thereby improve their predictive power as a whole. In one sense this has been successful - an order of magnitude more flows have been found - but in another, the set of flows gathered still falls short of that necessary to produce a good prediction. Extrapolating, it would seem an $O(10^8)$ long data set should yield $O(1000)$ recurrent flows which should provide an even better prediction but exactly how much better is unclear.

Over the rectangular torus, 2D Kolmogorov flow presents a number of interesting targets for recurrent flow analysis since the flow exhibits localised chaos in various different ways. Recurrent flow analysis has been applied to these flows (for the first time to undeniably transient flows) over a range of $Re$ with varying degrees of success. At $Re = 24$, the procedure has outperformed expectations with, in particular, just one recurrent flow proving a very good proxy for the chaos as in [12]. However, at larger $Re$ (here $\gtrsim 40$ for this extended domain), the picture quickly changes as it becomes more difficult to find nearly recurrent flows and even harder to convert these guesses into exactly recurrent flows. Given this, our results indicate that the early spectacular success of [12] was more a feature of the weakly (low-$Re$) chaotic nature of their small-box plane Couette flow than a reflection of the true situation in stronger chaos/turbulence.

Algorithmically, efforts have also been made to streamline the process of identifying nearly-recurrent flows since this procedure is very costly compared to only performing the DNS. Clearly there are some savings to be made, at least working in spectral space. Some preliminary calculations have also been performed with a recurrent check criterion performed in physical space. This was motivated by the efficiencies that should be present in focussing on a subdomain of the flow which contains the active dynamics. Although nothing could subsequently be converged here, this is surely a promising area for future work, especially when the lengthscale of observed (localised) coherent structures differs significantly from that of the full flow domain (e.g. as $Re$ increases). The one aspect of the recurrent flow analysis not investigated in any detail (except to adjust the various tolerances to help convergence) is the Newton-GMRES-Hookstep algorithm. Its behaviour is well known to be complex and only really understood when it is started ‘very’
close to an exact solution. Most importantly for the discussion at hand, it is possible for the algorithm to converge to a simple invariant set in a very different part of phase space than where it started. This is clearly undesirable as an initial guess embedded deep in the turbulent attractor can lead to a converged recurrent flow outside of the attractor and therefore irrelevant for any prediction. To avoid this scenario, a check could be instigated post-convergence to ensure the converged state is ‘close’ to the initial guess but this was not done here.

In terms of future directions, it should be clear that there are many challenges if the full programme of extracting recurrent flows directly from DNS data and then using them to predict turbulent statistics is to be pursued. Many will presumably be overcome, or at least reduced, by simply employing more computational power (e.g. the extraction of recurrent flows is readily automated). One outstanding question will, however, require more thought and perhaps a new idea/technique to emerge - how to weight the various contributions of the recurrent flows extracted. It seems highly probable that more (global) insight from phase space is needed to inform this process than just the (local) stability information of the recurrent flow. Finally, if one simply wants to obtain a preliminary understanding of the flow, extracting and scrutinising the structure of extracted recurrent flows buried in the flow provides valuable information about what closed cycles of dynamical processes underpin the chaos/turbulence. Just such an approach helped uncover the self-sustaining process [26] in wall-bounded shear flows following the discovery of a quasi-cycle in highly-constrained plane Couette flow [27]. This has not been a priority here due to the 2D nature of the flow but will be in a future report on a 3D version of Kolmogorov flow.

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APPENDIX A. RECURRENCE CRITERION

In section III A a considerable computational saving was achieved by reducing the number of modes included in the recurrence check. In this appendix we quantify such savings and the efficacy of alternative strategies. A series of shorter ($T = 2 \times 10^4$) DNS calculations on the $Re = 60$ attractor were performed each with a modified recurrence check. To establish how efficient the check was, attempts were also made to converge the guesses with the Newton-GMRES-hookstep algorithm. Applying this root-finding algorithm is by far the most computationally expensive component of the recurrent flow analysis so reducing the number of unconvergeable guesses has a significant impact on overall efficiency.

In the first investigation, the number of modes included in the recurrence check was varied starting with $8 \times 16$ (as in expression (15)), then using $32 \times 64$ (16 times as large) and comparing the results with $42 \times 84$ (the full state vector after de-aliasing) all with $R_{thres} = 0.3$. The results are outlined in table III which highlights the considerable overhead of the recurrence checking: the $8 \times 16$ case ‘only’ doubles the DNS runtime whereas the full resolution case completely swamps the basic DNS runtime.

In searching over all possible continuous shifts a discretisation of $2\pi$ must be employed with 30 shifts adopted as default following [6]. Increasing this figure to 120 discrete shifts resulted in more guesses and marginally more convergences but crucially entailed more computations: see table III. Interestingly, the more detailed recurrence check led to a different relative periodic orbit being converged (R56 from [6] with $T = 16.326$) instead of an orbit with $T = 17.975$ in the default case of 30 shifts from the same DNS data. This demonstrates clearly the sensitivity of the Newton-GMRES-hookstep algorithm to the initial guess.

The expression involving the full state vector is the obvious choice since it is precisely this residual which the Newton-GMRES attempts to converge to zero. However, it is not clear whether this criterion will be the most efficient at picking out guesses with higher likelihood of convergence; in other words recurrences which are more likely to be close passes to underlying unstable orbits. An alternative guess criterion was tested based upon the streamfunction ($\psi = \Delta^{-1} \omega$) which has the effect of producing a smoother field from which to define a recurrence. Computationally this simply amounts to replacing $\Omega$ in (15) with $\Psi = \Omega/|k|^2$, which effectively weights the small wavenumbers more heavily. Table III shows the results of this criterion (now with $R_{thres} = 0.07$ to pick out a comparable number of recurrences) and indicates a similar proportion of convergences; 31 out of 59 guesses, compared to 21 out of 42 for the default criterion. However, this new criterion was not only more computationally expensive (more operations computing $\Psi$) but also failed to converge any recurrences with $T > 5.0$ (how these criteria compare as $R_{thres}$ changes was not considered).

Finally, a two-fold strategy was tested to generate recurrent flow guesses. First, during the DNS, a norm of difference
in absolute value of the components:

\[
R(t, T) := \frac{\sum_{k_x=0}^{8} \sum_{k_y=-8}^{8} \left| \Omega_{k_x k_y}(t) \right|^2 - \left| \Omega_{k_x k_y}(t - T) \right|^2}{\sum_{k_x=0}^{8} \sum_{k_y=-8}^{8} \left| \Omega_{k_x k_y}(t) \right|^2}
\]  

(27)

was used as a necessary but not sufficient recurrence condition. This avoids the necessity to sweep over shifts, however, having generated a 'loose' guess in this fashion, there is a need to post-process to compute the necessary shifts before attempting convergence. For this reason, the CPU time quoted in table III includes the post-processing routine. This is a first attempt at a two-step strategy; we generated a large set of 'quasi'-guesses initially (2755) from which to process more accurate guesses. Due to the size of this set the post-processing took a considerable length of time, (257 CPU minutes) much longer in fact than the DNS. In retrospect, a smaller set of quasi-guesses and outputting both start and end points of the recurrence, would make this process more efficient. In any case, from 25 secondary guesses we converge only 5 recurrent flows. One has \( T > 5 \) and remarkably this is yet another new unique orbit which we have not found in any previous searches using the same DNS data.

| criterion          | # guesses | CPU time | factor | convergences |
|--------------------|-----------|----------|--------|--------------|
| DNS                | -         | 27.7     | -      | -            |
| \( 8 \times 16 \)  | 42        | 55.5     | 1      | 21           |
| \( 32 \times 64 \) | 35        | 456.2    | 8.2    | 16           |
| \( 42 \times 84 \) | 35        | 766.4    | 13.8   | 16           |
| \( N_s = 120 \)    | 69        | 138.5    | 2.5    | 25           |
| \( \psi \)         | 59        | 87.9     | 1.6    | 31           |
| \( |\Omega| \)      | 25        | 28.1 (+257) | 5.1      | 5            |

TABLE III. Table outlining successfulness of various recurrence checks and variants. First entry has DNS CPU time without recurrence checking for comparison, the following three show the standard check with various sizes (N.B. \( 42 \times 84 \) represents the full state vector), then standard check with higher fidelity \( s \) shift search, using the streamfunction \( \psi \) and final check is a residual based on absolute values of components. Using \( 8 \times 16 \) rather than the full \( 42 \times 84 \) gives a 13.8 times speed up.

**APPENDIX B**

In this appendix, details of all the recurrent flows found in section III are given in a table.

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TABLE IV. Table cataloguing the unstable recurrent flows extracted at $Re = 60$ Kolmogorov flow $n = 4$, $\alpha = 1$. Table shows period $T$, relative $x$-translation shift $s$, discrete $y$-shift $m$, inverse stability coefficient ($\Lambda^{-1}$, equation (17)), the number of unstable directions $N$, and the frequency with which the solution was converged (high is more than 20 and no frequency corresponds to a single convergence). Those prefixed with an ‘R’ are those already found in [6].
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