Referee's report:

'State space geometry of a spatio-temporally chaotic Kuramoto-Sivashinsky flow'

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The present manuscript concerns the Kuramoto-Sivashinsky (KS) equation, a model equation for complex dynamics in a deterministic PDE. There is already an extensive literature on this PDE, much of which discusses the apparently low-dimensional dynamical behavior and bifurcations displayed for relatively small system size L; while for large L this PDE is a much-studied example of spatio-temporal (extensive) chaos. The work under review is part of an ongoing program of the first author (Cvitanović) and his collaborators, dating back to Christiansen *et al.* (Ref. [3]), to identify (unstable) equilibria and periodic orbits, and to characterize chaotic and turbulent behavior as a "walk through the space of unstable patterns". A particular goal of this program has been the extension of periodic orbit (cycle) theory to infinite-dimensional dynamical systems (PDEs), to allow the computation of long-time averages of the chaotic dynamics via cycle expansions: appropriately ordered and weighted sums over periodic orbits; progress has included the development of algorithms to determine (a large number of) unstable periodic orbits and their properties.

While previous related work on the KS equation (Refs. [3, 22, 23]) was restricted to the subspace of odd solutions, which imposes strong constraints on the dynamics, in the manuscript under review this restriction has been lifted. Consequently, the system being studied has continuous as well as discrete symmetries, and a focus of this work is to study the effect of the continuous symmetries which permit, in addition to fixed points and periodic orbits, also *relative* equilibria and periodic orbits. The authors discuss symmetries and some associated dynamically significant invariant subspaces, identify and study equilibria and relative equilibria, and in particular compute many relative periodic orbits. They find interesting (but previously known) heteroclinic connections between some of the equilibria, and give examples of unstable (relative) periodic orbits which appear to resemble (in some representations) and yield similar averages to the observed chaotic dynamics.

The vision that "equilibria, relative equilibria, periodic orbits and relative periodic orbits ... form the repertoire of recurrent spatio-temporal patterns explored by turbulent dynamics" (p.22) is very appealing, but, in the light of the comments and concerns discussed below, unfortunately I do not feel that this manuscript yet provides sufficient evidence to support this conclusion. Thus, while I feel that this general research direction has much promise, I do not feel that I can recommend publication of this manuscript as it stands.

Some detailed comments:

- **Turbulence/Spatiotemporal Chaos/Chaos**

  A stated motivation for the present work is the understanding of the dynamics of turbulence; and the authors, following numerous precedents (for instance Ref. [16]), study the KS equation as a simpler model equation displaying some features relevant to turbulent flows. However, the authors fail to emphasize the significant differences between their model system and fully-fledged turbulence, or even spatiotemporal chaos (which has sometimes been labelled "weak turbulence" — see for instance the book by Manneville (1990)).

  On p.2 of this manuscript, it is stated that the terms "turbulence" and "spatiotemporal chaos" are used interchangeably; and both terms are used to describe to the dynamics of the $L = 22$ KS equation studied in this manuscript — $L = 22$ is claimed to be "the smallest system size for which KS empirically exhibits 'sustained turbulence' " (p.21). This seems to me not in accord with generally accepted usage: *turbulent* states (associated usually with fluid dynamics) are characterized by a range of scales and an energy cascade; *spatiotemporal chaos* (STC) refers to (large) extended systems with chaotic behavior characterized by a decay of spatial correlations, in which the attractor dimension and number of positive Lyapunov exponents diverges with system size L (see for instance Cross & Hohenberg, *Rev. Mod. Phys.* **65**, 851 (1993)). (My understanding is that to have STC, it is not sufficient merely to have chaotic temporal dynamics occurring in a PDE or other system with spatial dependence.) For the KS equation in the present scaling, STC occurs (roughly) for $L > 50 - 60$.

For the system size considered in the present manuscript, $L = 22$, on the other hand, the chaotic dynamics are low-dimensional, with a single positive Lyapunov exponent (p.10); there is no wide range of scales involved, nor decay of spatial correlations, and the system is not nearly in the extensively chaotic regime. Indeed, if one chooses slightly larger L, say $L = 25$, the KS dynamics are again attracted to a stable tri-modal equilibrium; and as shown for instance by Hyman, Nicolaenko & Zaleski, *Physica D* **23**, 265 (1986), there is a sequence of several more attracting fixed points, periodic and traveling wave solutions interspersed with chaotic behavior before the extensively chaotic regime is attained ($L = 22$ corresponds to α slightly larger than 49 in the scaling of Hyman *et al.*; see Fig. 1b of that paper).

In fact, it is proved (not "expected", as on p.10) that there is a finite-dimensional inertial manifold (see Ref. [9]; an upper bound on the dimension is given, for instance, in Jolly, Rosa & Temam, *Adv. Diff. Eqns.* **5**, 31 (2000)), which indicates that the dynamics are rigorously low-dimensional.

While the chaotic dynamics of such a relatively small KS system are of interest in their own right, I thus feel it is inappropriate to label this as "turbulent" or even "spatiotemporally chaotic" behavior, especially as for slightly larger L the chaotic dynamics disappear again. (For these reasons I also feel that the use of "spatio-temporally chaotic" in the title of this manuscript is incorrect.) Instead, I agree with the statement on p.22 that "much of the observed dynamics is specific to this unphysical, externally imposed periodicity. What needs to be understood is the nature of the equilibrium and relative periodic orbit solutions in the $L \to \infty$ limit ...".

On a related point: as motivation for the investigations of this manuscript, Fig. 2.1 of the present manuscript shows a typical spatiotemporally chaotic (not "turbulent") solution of the KS equation for $L \approx 89$; however, this is for a much larger system than the $L = 22$ system studied in this work. I feel that (instead of or in addition to Fig. 2.1) a representation of a "typical" chaotic solution for $L = 22$ should be shown, to facilitate comparison with trajectories such as those of the relative periodic orbits of Fig. 6.1.

- **Relative Periodic Orbits and Symmetries**
  In addition to the works cited (Refs. [14,20]), there is an extensive literature on equilibria, periodic orbits, and related solutions for the KS equation; thus I feel that more references to prior work, placing the investigations of this manuscript in the context of existing results on the dynamics, symmetries, geometry and bifurcations of small-L KS equations, would have been appropriate, especially to help clarify the contributions of the present work. For instance, the relevance of the $O(2)$ symmetries to the presence of heteroclinic orbits, and their importance in the overall dynamics, was first discussed by Armbruster, Guckenheimer & Holmes (*Physica D* **29**, 257 (1988), *SIAM J. Appl. Math.* **49**, 676 (1989); see also Refs. [16,20]); there is not much discussion of discrete symmetries other than D_2 in the work under review.

  Of particular interest in the present work are the relative periodic orbits, satisfying $u(x,t) = u(x + \ell_p, t + T_p)$; these are also known as *modulated traveling waves* (MTWs). These were studied, for instance, by Armbruster *et al.* (1988,1989), and a detailed computation of numerous bifurcation branches of these solutions was presented by Brown & Kevrekidis (in *Pattern*

Formation: Symmetry Methods and Applications, AMS, pp.45–66 (1996)), it would be of interest to know how the MTWs (relative periodic orbits) computed by the present authors for $L = 22$ fit into the complicated bifurcation structure discussed by Brown & Kevrekidis, as this might help in understanding them better.

In the manuscript under review, a large number of relative periodic orbits (MTWs) is computed for $L = 22$; however, the discussions concerning these MTWs and their dynamical significance (potentially the main contribution of this work) feel to me to be somewhat incomplete. For instance, a particular ("typical" — p.20) MTW with $T_p \approx 32.8$ is selected (Fig. 6.2(b)) which appears in the representations of Fig. 8.1 to be not too dissimilar from the chaotic (not "turbulent") flow. However, it is not fully discussed how generic this observation is: how was this orbit selected? What behavior would the other relative periodic orbits display? Is there a way to organize the relative periodic orbits, or to compute suitable averages over them? (I realize that much of this is the subject of ongoing research.)

- **Representation of Solutions**

  One of the stated main results of the present work is the visualization of the dynamics through "projections onto dynamically invariant, PDE-discretization independent state space coordinate frames", as well as through "physical, symmetry invariant observables, such as 'energy', dissipation rate, etc." (p.2).

  While it is apparent that eigenvectors of the equilibria E_1, E_2 and E_3 are dynamically invariant and relevant, it is not clearly discussed by the authors in which ways a visualization through projection onto these eigenvectors might have advantages compared to other previously-used approaches using, say, Fourier mode amplitudes. Indeed, a *representation* of the dynamics using, say, Fourier modes is quite independent of the *discretization* (finite difference, Galerkin, pseudo-spectral etc.) used for numerical integration of the PDE; and one could argue that Fourier modes (which are eigenvectors of the linearization about the trivial equilibrium E_0) are as dynamically relevant as eigenvectors of the other equilibria.

  If one is to follow the authors' suggestion to choose a representation using dynamical invariants, how does one choose a suitable set of axes? The authors do not seem to motivate, for instance, their choices of the stable eigenmodes Re $\mathbf{e}^{(6)}$ in Figs. 5.4 and 5.5, $\mathbf{e}^{(7)}$ in Fig. 5.6 and $\mathbf{e}^{(4)}$ in Fig. 5.8; other, apparently equally reasonable choices could have been made. Furthermore, their chosen representations vary from figure to figure, making comparisons between different figures difficult, as they contain eigenvectors of different equilibria. For instance (although this is not clearly discussed in the manuscript), the $\mathbf{e}^{(1)}$ of Figs. 5.4, 5.6 and 5.8 are all different, being the first unstable eigenmode of equilibria E_1, E_2 and E_3 respectively.

  It is also worthwhile to note that various authors (for instance Osinga) have already described three-dimensional visualizations of invariant manifolds. For the case of the KS equation, Johnson, Jolly & Kevrekidis, *Int. J. Bifur. Chaos* **11**, 1 (2001), demonstrate an interesting global bifurcation through visualization of changes in the geometry of the invariant manifolds.

  Energy

  As for the eigenmodes discussed previously, it is not really explained why projection onto axes of the (symmetry-invariant) energy, production and dissipation rates might be preferable to other means for visualizing solutions. (Note that in terms of the usual L^2 norm, these quantities defined on p.9 are merely $E = \|u\|^2/2L$, $P = \|u_x\|^2/L$, $D = \|u_{xx}\|^2/L$.) Indeed, I would expect that for spatially extended spatiotemporally chaotic or turbulent systems, much of the energy transfer would be localized in space, and could thereby not be captured by these spatially averaged measures. On the other hand, in the presence of sufficient spatial decorrelation (so that in the large-L limit, time averages of the chaotic dynamics may be approximated by spatial averages), I would expect as L increases, the difference between

$E(t)$, $P(t)$ and $D(t)$ and their time-averaged values would decrease, so that for larger L, a projection of solution trajectories onto E-P-D axes would become increasingly less useful.

- **Some smaller points include:**

  1. *Page 3:* There is a brief discussion here on the lack of structural stability with respect to truncation N, but I found little further indication in the remainder of the manuscript as to whether such sensitivity to N was indeed observed, or how the computed results were determined to be robust.
  2. *Page 6:* A clarification of the use of the term "GLMRT equilibrium" for E_1 might be helpful.
  3. *Page 9:* The first line of equation (3.8) should read
  $$\dot{E} = \langle u_t u \rangle = -\left\langle \left(u^2/2 + u_x + u_{xxx}\right)_x u \right\rangle .$$
  4. *Page 10:* In terms of the definition (3.6) for E in this manuscript, the best current bound (Refs. [1,12]) on $lim_{t\to\infty} E$ as a function of L scales as $E \propto L^2$, not $L^{3/2}$.
  5. *Page 12:* The last column of Table 5.1, for $\tau_{1/4}\mathrm{E}_n$ Symmetry, follows completely from the second-to-last column (under the exchange $\mathbb{U}^+ \leftrightarrow \mathbb{U}^{(1)}$), and thus seems redundant. Why do many, but not all, of the eigenvalues of E_3 come in pairs?
  Are the eigenvalues of $\mathrm{TW}_{\pm 1}$ and $\mathrm{TW}_{\pm 2}$ plotted in Fig. 5.2, as indicated in the text?
  6. *Page 13:* While I was able to compute the values of T for E_1 and E_2 in Table 5.2 according to the prescription of p.12, I do not understand how $T \approx 10.71$ as the characteristic time scale for E_3 was computed.
  There is considerable discussion of the dynamical relevance of the unstable manifolds of the equilibria, but appears to be none concerning the relative equilibria (traveling waves) shown in Fig. 5.3; can anything be said regarding their influence on the dynamics?
  7. *Page 15:* I found no reference to Figure 5.7 in the text.
  In the caption of Fig. 5.6: the eigenvector $\mathbf{e}^{(7)}$ for E_2 seems to be complex (see Table 5.1), so surely one needs to choose either Re $\mathbf{e}^{(7)}$ or Im $\mathbf{e}^{(7)}$?
  In the paragraph below Fig. 5.6: Not all orbits within the unstable manifold of E_2 converge to $\tau_{1/4}$ E_2, since there is a trajectory approaching E_3.
  8. *Page 16:* Some more discussion in the text with computational details concerning how the search for relative periodic orbits was performed, or stronger references to the Appendices, might be useful in Section 6.
  9. *Appendices:* The motivation for including these appendices should be made clearer; could it have been sufficient just to cite Refs. [18, 24] and other references for the algorithms? (Note that Brown & Kevrekidis (1996) also give an algorithm for computing MTWs (relative periodic orbits)). It was also not clear to me whether the Levenberg-Marquardt search of App. C or the Newton shooting method of App. D was used for these computations. It would be helpful to have an indication of how these two methods compare, and which might be preferable.
  Some care might be taken with notation. For instance, a_p in (C.1) refers to a vector of $N-2$ Fourier modes, while a_k in (2.2), p.3 is an individual Fourier mode, and a_0 near the bottom of p.24 is a starting guess (is $a_0 = a^{(1)}$ in (C.2)?).
  The definitions of a, T and ℓ could have been written in App. C, rather than just being given at the beginning of App. D.