Spatiotemporal tiling of the Kuramoto-Sivashinsky flow

Matthew N. Gudorf, and Predrag Cvitanović,

Abstract. a new spatiotemporal formulation to provide a new perspective. 1 2

The main goal of this reformulation is to provide a qualitative and quantitative description of the infinite space-time behavior of the Kuramoto-Sivashinsky flow.

Advances in experimental imaging, computational methods, and dynamical systems theory reveal that the unstable recurrent flows observed in moderate Reynolds number turbulent flows result from close passes to unstable invariant solutions of Navier-Stokes equations. In past decade hundreds of such solutions been computed for a variety of flow geometries, always confined to small computational domains (minimal cells). While the setting is classical, such classical field-theory advances offer new semi-classical approaches to quantum field theory and many-body problems.

The Gutkin and Osipov on many-particle quantum chaos (in particular, the spatiotemporal cat lattice models) suggests a path to determining such solutions on spatially infinite domains. Flows of interest (pipe, channel flows) often come equipped with D continuous spatial symmetries. If the theory is recast as a (D+1)-dimensional space-time theory, the space-time translationally recurrent invariant solutions are (D+1)-tori (and not the 1-dimensional periodic orbits of the traditional periodic orbit theory). Spatiotemporal cat lattice models suggest that symbolic dynamics should likewise be (D+1)-dimensional (rather than a single temporal string of symbols), and that the corresponding zeta functions should be sums over tori, rather than 1-dimensional periodic orbits.

Key words. relative periodic orbits, chaos, turbulence, continuous symmetry, Kuramoto-Sivashinsky equation

AMS subject classifications. 35B05, 35B10, 37L05, 37L20, 76F20, 65H10, 90C53

1. Introduction. Recent experimental and theoretical advances [20] support a dynamical vision of turbulence: For any finite spatial resolution, a turbulent flow follows approximately for a finite time a pattern belonging to a finite alphabet of admissible patterns. The long term dynamics is a walk through the space of these unstable patterns. The question is how to characterize and classify such patterns? ³ Chaotic nonlinear systems constitute one of the few classical physics problems yet to be solved. The behaviors exhibited are so peculiar that it has permeated into popular culture via the butterfly effect. This behavior poses a serious challenge which has effects everything from weather prediction to air travel. In the recent past computational successes were made by studying turbulent flows on minimal cells: small domains that could support turbulence and remain computationally tractable. These successes came in form of time invariant solutions alkso known as "exact coherent structures" (ECS) [33, 35]. These solutions are important because it is their unstable and stable manifolds that dictate the dynamics [2]. Not only have conventional methods not worked on large domains, we argue that they never could have worked. The motivation behind minimal cells was to develop an intuition for turbulence which would be used to obtain results on progressively

^{*}School of Physics, Georgia Institute of Technology, Atlanta, GA 30332-0430, USA

¹Matt 2019-03-15: An example of me commenting; magenta text marks my edit.

²Predrag 2019-05-13: In [6] equation numbers are on the right; here they are on the left. Check a recent issue of SIADS, fix this or not, and move this question, answered, to Sect. 8.

³Matt 2020-01-20: [Background]

large domains.

In light of all of these difficulties we believe that new bold ideas are required to resume forward progress. We retreat from the conventional wisdom to start anew with a truly spatiotemporal theory, one that treats infinite space-time as the shadowing of a finite number of fundamental patterns which we denote as "tiles".

⁴ The primary claim that we make is that in hindsight, describing turbulence via an exponentially unstable dynamical equation never could have worked. Conventional methods treat spatial dimensions as finite and fixed and time as inherently infinite. Our spatiotemporal formulation of chaos treats all continuous dimensions with translational invariance democratically as (1+D) different 'times'. The proposal is inspired by the Gutkin and Osipov [18] modelling of chain of N coupled particle by temporal evolution of a lattice of N coupled cat maps.

The alternative that we propose to describe infinite space-time chaos via the shadowing of fundamental patterns which we refer to as "tiles". These tiles are the minimal "building blocks" of turbulence; they are realized as doubly-periodic orbits which are global solutions with compact support. Finding the tiles of turbulence is fundamentally easier than finding doubly-periodic orbits on larger domains due to the exponential growth in complexity of solutions. In other words there are fewer important solutions on smaller domains. This in turn implies that there can only be a small number of fundamental tiles. This is what makes the problem tractable: if we can collect the complete set of tiles then we have the ability to construct every doubly-periodic orbit according to our theory.

The lack of exponentially unstable dynamics has powerful and immediate effects. Because there is no time integration, the problem of finding doubly-periodic orbits is now a variational one. The benefit of this is that there is no need to start an initial guess on the attractor; the optimization process handles this entirely. This allows us to find arbitrarily sized doubly-periodic orbitsbut in fact there is no need to. Our hypothesis is that we need only to find the building blocks which shadow larger doubly-periodic orbits and infinite space-time.

The spatiotemporal formulation allows a much easier categorization of what is "fundamental" by virtue of the frequency that patterns admit in the collection of doubly-periodic orbits. By identifying the most frequent patterns, we shall clip these patterns out of the doubly-periodic orbits they shadow and use them as initial conditions to search for our tiles.

The notion of "building blocks of turbulence" is one of the reasons for studying fluid flows in the first place. There is evidence that certain physical processes are fundamental, but they have yet to be used in a constructive manner. The spatiotemporal description is able to actually put these ideas in practice. The spatiotemporal completely avoids this by constructing larger doubly-periodic orbits from the combination of smaller doubly-periodic orbits. The reason why the search for the fundamental tiles is classified as "easy" is because in the small domain size limit there just aren't that many doubly-periodic orbits; the dynamics is relatively simple.

The first key difference is that the governing equation dictates the spatiotemporal domain size in an unsupervised fashion. The results here are not The only reason why L was treated as fixed is due to the inherent instability it includes when treated as a varying quantity. This

⁴Matt 2020-01-20: [Revolution] WHY?

small detail, allowing the domain size L to vary, is not as trivial as it seems. This difficulty is especially evident in the Kuramoto-Sivashinsky equation, whose spatial derivative terms are of higher order than the first order time derivative, but also there is a spatial derivative present in the nonlinear component.

Specifically, we propose to study the evolution of Kuramoto-Sivashinsky on the 2-dimensional infinite spatiotemporal and develop a 2-dimensional symbolic dynamics for it: the columns coding admissible time itineraries, and rows coding the admissible spatial profiles. Our spatiotemporal method is the clear winner in both a computational and theoretical sense. By converting to a tile based shadowing description we have essentially removed the confounding notion of an infinite number of infinitely complex doubly-periodic orbits from the discussion. Now we must put these ideas into practice. The testing grounds for these ideas will be the spatiotemporal Kuramoto-Sivashinsky equation

(1.1)
$$u_t + u_{xx} + u_{xxx} + uu_x = 0$$
 where $x \in [0, L], t \in [0, T]$

where u=u(x,t) represents a spatiotemporal velocity field. This equation has been used to model many different processes such as the laminar flame front velocity of Bunsen burners. While (1.1) is much simpler than the spatiotemporal Navier-Stokes equation, we would argue that the main benefit is the simplicity of visualizing its two-dimensional space-time. This visualization makes the arguments more understandable and compelling in addition to making the tiles easier to identify. The translational invariance and periodicity of (1.1) make spatiotemporal Fourier modes a natural choice. The inherently infinitely dimensional equations are approximated by a Galerkin truncation of these spatiotemporal Fourier modes. The Kuramoto-Sivashinsky equation (1.1) in terms of the Fourier coefficients $\hat{\bf u}$ is a system of differential algebraic equations $\hat{\bf u}$

(1.2)
$$F(\hat{\mathbf{u}}, L, T) \equiv (\omega - k^2 + k^4)\hat{\mathbf{u}} + \frac{k}{2}\mathcal{F}(\mathcal{F}^{-1}(\hat{\mathbf{u}})^2).$$

The nonlinear term is computed in a pseudospectral fashion: a method which computes the nonlinear term as a product in physical space as opposed to a convolution in spectral space. The definitions of each term is as follows; \mathcal{F} and \mathcal{F}^{-1} represent the forward and backwards spatiotemporal Fourier transform operators. Likewise, ω and k contain the appropriate temporal and spatial frequencies to produce the corresponding derivatives. Any and all indices are withheld to avoid unnecessary confusion at this stage. The spatiotemporal system of differential algebraic equations (1.2) is of the form $F(\hat{\mathbf{u}}, L, T) = 0$. This type of optimization problem is ubiquitous in engineering and optimization literature. Therefore solving (1.2) is a matter of adapting known numerical methods to its idiosyncracies. Once we have the ability to solve (1.2) we need to first create a collection of doubly-periodic orbits. The only requirement that the collection must satisfy is that it must capture all fundamental patterns by adequately sampling the set of doubly-periodic orbits. In other words an exhaustive search is not our aim; not only that, but also the collection need not sample all spatiotemporal domain sizes. We hypothesize that there is some upper bound on the spatiotemporal size of fundamental tiles due to spatiotemporal correlation lengths. Once the collection is deemed sufficient we proceed to visual inspection. In this manner we determine the most frequent patterns and single them out as tile candidates. This is done by literally clipping them out of the doubly-periodic orbits that they shadow. Each clipping is then treated as an initial guess for a fundamental tile which is itself a doubly-periodic orbit. Therefore, these represent initial conditions for the optimization method. It is not a guarantee that every clipping converges to a doubly-periodic orbit; therefore the number of attempts to find a tile should continue until it does in fact converge. The number of convergence attempts is typically proportional to how confident we are that the pattern being scrutinized is in fact a tile. Once a collection of tiles is collected, we can construct new and reproduce known doubly-periodic orbits. This is completed with a method we refer to as "gluing". It is as straightforward as one might infer: tiles are combined in a spatiotemporal array to form initial conditions used to find larger doubly-periodic orbits. Methods of gluing temporal sequences of doubly-periodic orbits exist but never has the ability to glue doubly-periodic orbits spatiotemporally existed before. With the implementation of the gluing method can begin to probe the 2-dimensional spatiotemporal symbolic dynamics previously mentioned. A fully determined symbolic dynamics is sufficient to describe infinite space-time completely. We already have the two edges of this symbol plane - the L=22 minimal cell [6, 25] is sufficiently small that we can think of it as a low-dimensional ("few-body" in Gutkin and Klaus Richter [8, 7, 9, 10] condensed matter parlance) dynamical system, the left-most column in the Gutkin and Osipov [18] 2D symbolic dynamics spatiotemporal table (not a 1-dimensional symbol sequence block), a column whose temporal symbolic dynamics we will know, sooner or later. Michelson [28] has described the bottom row. The remainder of the theory will be developed from the bottom up, starting with small spatiotemporal blocks.

The plans for our spatiotemporal formulation have been laid bare. The main concept is that the infinities of turbulence can be described by spatiotemporal symbolic dynamics whose letters are fundamental spatiotemporal patterns. Consequentially, we have created numerical methods which not only perform better than conventional methods but also present incredible newfound capabilities. These newfound capabilities include but are not limited to finding small doubly-periodic orbits which shadow larger doubly-periodic orbits but also constructing larger doubly-periodic orbits from smaller ones. These new and robust methods alone present a way forward for turbulence research, hence their is merit in a spatiotemporal formulation even though the theory has not been fully fleshed out. To test our spatiotemporal ideas we require three separate numerical methods: the first should be able to find doubly-periodic orbits of arbitrary domain size. The second needs to be able to clip or extract tiles from these doubly-periodic orbits. Lastly, we need a method of gluing these tiles together. All three of these techniques require the ability to solve the optimization problem $F(\hat{\mathbf{u}}, T, L) = 0$ on an arbitrarily sized doubly periodic domain.

⁵ As previously discussed, this work does not use approximate recurrences or time integration to generate initial conditions. Instead we simply initialize a lattice of Fourier modes by first deciding on the dimensions of the lattice and then assigning random values to the modes. Specifically, random values in this case are drawn from the standard normal distribution and then normalized such that the physical field u(x,t) has the assigned maximum value. Manipulations of the Fourier spectrum can also be made but we have no specific recommendation for how to do so as it can be rather unintuitive.

⁵Matt 2020-02-18: How?

The first method substitutes an equivalent optimization problem instead of directly solving F = 0. The optimization problem is formed by the construction of a scalar cost function

(1.3)
$$\mathcal{I}(\hat{\mathbf{u}}, T, L) = \frac{1}{2} ||F(\hat{\mathbf{u}}, T, L)||_2^2.$$

taking a derivative with respect to a fictitious time τ

$$\frac{\partial \mathcal{I}}{\partial \tau} = \nabla \left(\frac{1}{2} ||F(\hat{\mathbf{u}}, T, L)||_{2}^{2} \right) \partial_{\tau} [\hat{\mathbf{u}}, T, L]
= \left(\left[\frac{\partial F}{\partial \hat{\mathbf{u}}}, \frac{\partial F}{\partial T}, \frac{\partial F}{\partial L} \right]^{\top} F(\hat{\mathbf{u}}, T, L) \right) \cdot \partial_{\tau} [\hat{\mathbf{u}}, T, L]
\equiv \left(J^{\top} F \right) \cdot \partial_{\tau} [\hat{\mathbf{u}}, T, L] \quad .$$
(1.4)

This equation (1.4) by itself does not provide us with a descent direction because $\partial_{\tau}[\hat{\mathbf{u}}, T, L]$ remains unspecified. The simplest choice is the negative gradient of the cost function; this choice corresponds to the gradient descent algorithm.

(1.5)
$$\partial_{\tau}[\hat{\mathbf{u}}, T, L] = -\left(J^{\top} F\right),$$

such that

(1.6)
$$\frac{\partial \mathcal{I}}{\partial \tau} = -\left\| \left(J^{\top} F \right) \right\|_{2}^{2} \le 0.$$

In order to "descend" we use Euler's method to integrate in the descent direction. Note that this integration is with respect to fictitious time and represents making successive variational corrections; it is not dynamically unstable time integration. We elect to use a combination of step limit and absolute tolerance to determine when the descent terminates. If the cost function doesn't cross the threshold by the step limit then the descent is terminated. The descent algorithm can be viewed as a method of converging approximate solutions close enough to a final doubly-periodic orbit such that the least-squares algorithm can converge them, akin to [11].

The second method is application of a least-squares solver to the root finding problem F = 0. The Newton system is derived here for context.

(1.7)
$$F(\hat{\mathbf{u}} + \delta \hat{\mathbf{u}}, T + \delta T, L + \delta L) \approx F(\hat{\mathbf{u}}, T, L) + J \cdot [\delta \hat{\mathbf{u}}, \delta T, \delta L] + \dots$$

substitution of zero for the LHS (the root) yields

(1.8)
$$J \cdot [\delta \hat{\mathbf{u}}, \delta T, \delta L] = -F(\hat{\mathbf{u}}, T, L).$$

where

(1.9)
$$J \equiv \left[\frac{\partial F}{\partial \hat{\mathbf{u}}}, \frac{\partial F}{\partial T}, \frac{\partial F}{\partial L} \right].$$

Technically this equation is solved iteratively, each time producing its own least-squares solution which guides the field to doubly-periodic orbit. The equations are augmented to include

variations in T, L and as such the linear system is actually rectangular. We chose to solve the equations in a least-squares manner as we are not focused on finding a unique solution; any member of a doubly-periodic orbits group orbit will do. The price of this indefiniteness is that we might collect doubly-periodic orbits which belong to the same group orbit. To improve the convergence rate of the algorithm we also include backtracking: the length of the Newton step is reduced until either a minimum length is reached (failure) or the cost function decreases. As a caveat, our specific least-squares implementation is memory limited. That is, we can only apply it to some maximum dimension as it requires the explicit construction of a large, dense matrix. Currently it suits our purposes such that we do not include any other numerical methods in this discussion. The primary numerical methods that we apply have been described. Now we can move onto describing exactly how we used these method to further our spatiotemporal theory.

As previously mentioned, we must first find a collection of doubly-periodic orbits which we believe adequately samples the space of doubly-periodic orbits, up to some maximum size. We automated the search over a range of periods and domain sizes. Periods were chosen from the range $T \in [20, 180]$. Meanwhile, the spatial range was $L \in [22, 88]$. The discretization size depended on the spatiotemporal domain size; more modes are needed to resolve larger solutions. The number of lattice points in each dimension were typically chosen to be powers of two in order because of their interaction with discrete Fourier transforms. A strict rule for lattice size was never developed so we offer is the approximate guidelines

(1.10)
$$M = 2^{\inf(\log_2(L) + 1)}$$

for space and

(1.11)
$$N = 2^{\inf(\log_2(T))}.$$

for time. The tolerance of the cost function for the gradient descent was typically set at 10^{-4} and the step limit was set as a function of the size of the lattice. For the least-squares with backtracking the tolerance for termination was originally 10^{-14} and the step limit was 500. The large step limit was because of the allowance of back-tracking, which reduces the step length. The final tolerance can likely be relaxed as there is minimal change in solutions over many orders of magnitude of the cost function; an indication that a different norm should be used. As a reminder, our claim is that the tiles are doubly-periodic orbits which shadow larger doubly-periodic orbits. Therefore we should be able to converge subdomains which have been numerically clipped out of larger doubly-periodic orbits. After visual inspection, we believed the number of fundamental tiles to be small. Therefore, a precise and unsupervised algorithm for clipping was not developed. Instead the only criteria we abided by is that the clipping must include the tile being sought after; of course, clippings that were closer to being doubly periodic were sought after. For the original doubly-periodic orbit with dimensions $x \in [0, L_0]$ and $t \in [0, T_0]$ defined on a lattice, the clipping can be described as follows. Find the approximate domain on which the shadowing occurs and then literally extract the subregion of the parent lattice, setting the new spatiotemporal dimensions according to the smaller lattice. In other words, the same grid spacing was maintained throughout this procedure. This process in combination with our numerical methods was sufficient for finding tiles. It is one thing to claim that certain spatiotemporal doubly-periodic orbits are the building blocks of turbulence for the Kuramoto-Sivashinsky equation. It is another thing entirely to put our money where our mouth is by actually using them in this manner. We would like to remind the audience that the ability to construct and find solutions in this manner has not been witnessed in the literature. With this in mind our choices should be treated as preliminary ones; it is entirely possible and likely that many improvements could be made. Much like the clipping process used to find tiles combining solutions in space-time, the overarching idea of gluing is straightforward and intuitive. Specifically, the tiles represent the Brillouin zone, fundamental domain, unit cell of a lattice, etc. of each fundamental doubly-periodic orbit. The general case is that we have a general $s_n \times s_m$ sized mosaic of tiles. The admissibility of the gluing is determined by the (currently unknown) symbolic dynamics. Gluing is only well defined if the lattices being combined have the same number of grid points along the gluing boundary. This creates a problem, however, as different tiles will have different spatiotemporal dimensions T, L because they are fundamentally different solutions. This actually helps provide a precise meaning to the term "gluing". Gluing is a method of creating initial conditions which approximates a non-uniform rectangular lattice (combination of tiles) as uniform. This of course introduces local error which depends on the grid size; therefore there should not be an extreme discrepancy between the doubly-periodic orbits or tiles being glued. With this in mind, we simply rediscretize and concatenate the new lattices. The dimensions of the new lattice are determined by the sum or average of the original dimensions. For example, if gluing two tiles together in time, the new period would be $T = T_1 + T_2$ but the new spatial period is $L = \frac{L_1 + L_2}{2}$. In this case the number of spatial grid points and temporal grid spacing should be the same. There are many more complicated alternatives, limited only by the imagination.

2. OLD: Introduction. For a subset of physicists and mathematicians who study idealized 'fully developed,' 'homogenous' turbulence the generally accepted usage is that the 'turbulent' fluid is characterized by a range of scales and an energy cascade describable by statistic assumptions [13]. What experimentalists, engineers, geophysicists, astrophysicists actually observe looks nothing like a 'fully developed turbulence.' In the physically driven wall-bounded shear flows, the turbulence is dominated by unstable *coherent structures*, that is, localized recurrent vortices, rolls, streaks and like. The statistical assumptions fail, and a dynamical systems description from first principles is called for [21].

Dynamical state space representation of a PDE is ∞ -dimensional, but the Kuramoto-Sivashinsky flow is strongly contracting and its non-wondering set, and, within it, the set of invariant solutions investigated here, is embedded into a finite-dimensional inertial manifold [12] in a non-trivial, nonlinear way.

'Tiling' in the title of this paper refers to our attempt to systematically triangulate this set in terms of dynamically invariant solutions (equilibria, periodic orbits, ...), in a PDE representation and numerical simulation algorithm independent way.

If we ban the words 'turbulence' and 'spatiotemporal chaos' from our study of small extent systems, the relevance of what we do to larger systems is obscured. The exact unstable coherent structures we determine pertain not only to the spatially small 'chaotic' systems, but also the spatially large 'spatiotemporally chaotic' and the spatially very large 'turbulent' systems. So, for the lack of more precise nomenclature, we take the liberty of using the terms

'chaos,' 'spatiotemporal chaos,' and 'turbulence' interchangeably.

MERGE IN: leads to what, in the context of boundary shear flows, would be called [19] the 'empirically observed sustained turbulence,' but in the present context may equally well be characterized as a 'chaotic attractor.'

Asymptotic attractor structure of small systems like the one studied here is very sensitive to system parameter variations, and, as is true of any realistic unsteady flow, there is no rigorous way of establishing that this 'turbulence' is sustained for all time, rather than being merely a very long transient on a way to an attracting periodic state.

In previous work, the state space geometry and the natural measure for this system have been studied [4, 24, 25] in terms of unstable periodic solutions restricted to the antisymmetric subspace of the Kuramoto-Sivashinsky dynamics.

The focus of [6] was on the role continuous symmetries play in spatiotemporal dynamics. The notion of exact periodicity in time is replaced by the notion of relative spatiotemporal periodicity, and relative equilibria and relative periodic orbits here play the role the equilibria and periodic orbits played in the earlier studies.

There is a vast literature on relative periodic orbits since their first appearance, in Poincaré study of the 3-body problem [3, 30], where the Lagrange points are the relative equilibria. They arise in dynamics of systems with continuous symmetries, such as motions of rigid bodies, gravitational N-body problems, molecules, nonlinear waves and the plane Couette fluid flow [31].

In presence of a continuous symmetry any solution belongs to a group manifold of equivalent solutions. The problem: If one is to generalize the periodic orbit theory to this setting, one needs to understand what is meant by solutions being nearby (shadowing) when each solution belongs to a manifold of equivalent solutions. In [29] we resolve this puzzle by implementing symmetry reduction.

3. Results.

4. Transition and summary so far. So far we have motivated a spatiotemporal theory of turbulence which replaces unstable dynamics with spatiotemporal patterns. We formulated these ideas using the Kuramoto-Sivashinsky equation and then described a few methods with which to solve the corresponding equations. The following section describes the results of our numerical investigation.

5. Results.

5.1. Library Results.

5.1.1. Solution and Noise. The first application of our numerical methods was to coarse spatiotemporal discretizations of known solutions. Indeed, these solutions converged to doubly-periodic orbits, with slightly different spatiotemporal domain size because it is no longer fixed. Next we tested how robust the spatiotemporal topology is by adding noise to the newly spatiotemporally converged doubly-periodic orbits. While we believed that the topology would be robust to noise, the extent to which this is true was surprising. Specifically the noise that doubly-periodic orbits could withstand is larger than the magnitude of the original field itself. Specifically, the additive noise was an *aperiodic* lattice of values drawn from the standard normal distribution multiplied by the L_{∞} norm of the solution's field. The sum of these two

fields converged to a nearly identical solution after taking domain changes and symmetry operations into account.

- **5.1.2.** How the search progressed. The robustness to noise was an encouraging start to the search for spatiotemporal solutions. The next step was to attempt to converge solutions generated in the manner prescribed in Sect. ??. The search included simple symmetries whose initial domain sizes sampled $L \times T \in [22, 66] \times [20, 200]$. The computation time depends on the dimension of the lattice which in turn depended on the domain size such that it is hard to give an approximate runtime for each trial. By fine tuning the search according to different factors such as domain size, numerical method parameters, etc., produced a library of a few thousand solutions within a relatively short period of time. First, we provide the reader with some sample initial conditions and the solutions that they converged to. This is important as we believe this depicts the numerical strength of the spatiotemporal formulation.
 - 5.1.3. Analysis of the library.
 - **5.1.4. Outliers.** Within our collection of solutions
 - 5.2. Tile results.
- **5.2.1.** Identification of tiles from large trajectory. Analysis of our library of solutions allowed us to formulate guesses as to which spatiotemporal patterns represented fundamental tiles. Specifically we made a handful of guesses based on spatiotemporal frequency and spatiotemporal domain size. With only our crude intuition guiding us we restricted our search to patterns that involved at most two wavelengths $L/(2\pi) = \tilde{L} \approx 2$. Some of these guesses were aperiodic, requiring the inclusion of spatial translation symmetry in order to begin the search.
- **5.2.2. Clippings.** The search for tiles then began by clipping these guesses out of known solutions. The majority of the tiles were found by single-step clippings as opposed to the iterative method described in Sect. ??. Regardless, we find it informative to provide figures of both in (). The hardest clippings to converge by far were the guesses with continuous symmetry. This was presumably due inherent aperiodicity of each guess as the spatial shift was sensitive to discontinuities at the boundaries in time.
- **5.2.3. Converged tiles.** The tile solutions agree with our guesses in the sense that the final pattern is approximated by the original guess. In addition, each tile represents a simple physical process that allows us to name and give precise meaning to each tile.

This collection of fundamental tiles contains information on the intrinsic physical scales to our problem.

5.2.4. Continuous families. Before we disseminate the results of our tile search, we must first discuss a detail essential to the spatiotemporal theory. This realization came as a byproduct of the tests regarding noise previously described in (). These tests imply that solutions exist in families defined by continuous deformations of domain size and field values. By itself this is not shocking; it is equivalent to solution branches in bifurcation analyses. When combined with the notion of symbolic tiles, however, it essentially defines our theory and the way forward. In essence it says that our symbolic tiles do not form a discrete alphabet as originally

presumed. Instead, our tiles are rubber, such that each tile in a 2-dimensional spatiotemporal symbolic block requires a specification of the size of each tile. Another interpretation is that every solution exists in a continuous family of solutions because the tiles exist in continuous families. This betrays our intuition because in hyperbolic systems solutions are isolated from one another due to their unstable manifolds. While this is a great result in a practical sense, it leaves us with many open theoretical questions as described in Sect. 7. Exploration of these continuous tile families benefited us greatly. It turns out that a number of our tiles were in fact realizations of the same tile on different domain sizes. This in turn reduced our unique tile collection down to three tiles (three continuous families, technically). This in turn implies that the complexity of infinite space-time of the Kuramoto-Sivashinsky equation can be described by three patterns and their combinations, a result that exceeded our expectations.

- **5.3.** Gluing results. Our claim is that only three tiles are required to describe the Kuramoto-Sivashinsky equations infinite space-time. If this claim is true, then all solutions can be described by the spatiotemporal combination of these tiles. Note that the converse is not necessarily true; inadmissible combinations of tiles will form what is known as the grammar of our spatiotemporal symbolic dynamics. To test this claim, we need to combine tiles together and converge them to solutions. Before we begin with this explicitly, we provide results that demonstrate the same behavior but with known solutions (which are not fundamental tiles).
- **5.3.1. Time gluing.** The first demonstration of this idea is the combination of doubly-periodic orbits only with respect to time. This is essentially a spatiotemporal method to produce the familiar temporal itineraries required for temporal symbolic dynamics in periodic orbit theory.
- **5.3.2. Space gluing.** Just as we can glue in time, we can now glue in space. While just as intuitive as gluing in time, we have not observed anyone attempt a similar method. Much like clipping, gluing need not be done in a single step, rather, it can also be performed iteratively.

5.3.3. Repeated spatial gluing.

- **5.3.4. Tile combinations.** With our demonstrations of temporal and spatial gluing in place, we finally arrive at perhaps the most enticing results. Namely, we can now glue tiles in a spatiotemporal manner.
- **5.3.5.** Reproduction of target solution. As a first test our of claim that tiles combinations constitute all solutions, we design an initial condition from our tiles that, once converged, reproduces a known solution. This was a proof of concept; as such, it included using specific members of the tile families to reproduce the solution.
- **5.3.6.** New solutions. With this test in mind, we can see if perhaps we can automate this process to produce arbitrary solutions. In other words, we replace the specifically tailored tiles used in the previous example with static representatives of each tile family. As shown in the exploration of each continuous family, it is likely best to utilize intermediate family members away from the boundaries of the domain.

Much like how we did not need to exhaust the entire space of doubly-periodic orbits to determine our tiles, exhausting all tile combinations to determine our grammar is perhaps not

necessary. This is a very speculative claim that is only based on our intuition which honestly speaking, has been wrong at nearly every stage of the game.s

6. Summary.

- **6.1. Summary.** We have put for a spatiotemporal formulation of turbulence which replaces exponentially unstable dynamics for a collection of fundamental spatiotemporal patterns. There is evidence that arbitrary spatiotemporal solutions can be described by combinations of these special doubly-periodic orbits, which we denote as "tiles". Additionally, preliminary investigations support the claim that only three tiles are required for these spatiotemporal constructions. Our results were made possible by the implementation of numerical methods which are robust due to topological considerations. This lead to newfound capabilities and techniques that so far have not been witnessed elsewhere. Specfically, by allowing the entire spatiotemporal domain to vary during the optimization process we are able to extract small doubly-periodic orbits from larger doubly-periodic orbits(clipping) as well as build large doubly-periodic orbits by combining smaller doubly-periodic orbits(gluing). The latter of these two techniques is very powerful as it allows us to find doubly-periodic orbits of progressively larger spatiotemporal extent. Not only that, it acts as a staging ground for the determination of a 2-dimensional spatiotemporal symbolic dynamics.
- **6.2. Open Challenges and Future work.** Our techniques, if they can be applied to the Navier-Stokes equations, would allow for the construction of larger spatiotemporal solutions using the known exact coherent structures defined on minimal cells. While the spatiotemporal "tiles" of the Navier-Stokes equations are not currently known, there is much more intuition as to what physical processes are fundamental; it is our hope that this knowledge can be leveraged to find the four dimensional space-time tiles. With these new ideas come an amalgam of fundamental questions, most of which have yet to be unanswered.
- 6.2.1. Theory of tile families, rubberized, tiles identified globally, not localized. The most important open question is how to realize a 2-dimensional spatiotemporal symbolic dynamics in the face of continuous tile families. If we are lucky, admissibility is not dependent on the size of the tiles but merely their spatiotemporal configurations (and possibly symmetry considerations). It is of course always possible that the admissibility depends on the family in a (fractal?) manner. Another unfortunate detail is that the grammar could be obfuscated by the potency numerical methods; in other words, a symbolic combination may be admissible but the specific numerical methods employed might not be able to find it. Almost assuredly better numerical methods exist as the ones currently employed are towards the simple end of the complexity continuum. The lack of description of the symbolic dynamics also leaves much to be desired in terms of the implementation of the gluing method. There are a number of important details not yet considered which prevent us from implementing a systematic gluing method. Three examples are: including tile-wise local Galilean velocities, continuous tile family considerations, as well as symmetry considerations. The guiding principal would be to minimize the extent of the discontinuities at the tile boundaries. We know that each tile will locally solve the Kuramoto-Sivashinsky equation on their interior such that the effect of solving the gluing optimization problem is mainly to smooth out these discontinuities.

- **6.2.2.** Have no metric to tell if final tile is the realization of the symbolic initial condition. For every gluing combination, it is essential (for the grammar) that the result be a realization of the initial symbolic combination. It is possible (and believed to happen very often) that the gluing combinations converge to the "wrong" doubly-periodic orbits. Currently, we have no notion of topological signatures or topological invariants that could be used to validate our results.
- **6.2.3. no physical predictions yet.** The lack of a systematic gluing method and symbolic dynamics prevents us from predicting or calculating any physical quantities.
- **6.2.4.** Navier-Stokes or Kolmogorov or spiral waves. As a reminder, this was a testing ground for these ideas. The main goal is to eventually apply this to systems which are physically realizable. This requires a large amount of effort that will hopefully be reduced by collaborative efforts once the research code is released to the public.
- **6.2.5.** Subdivision of domain; can't use Fourier. Another potential and perhaps necessary component of the spatiotemporal formulation is the ability to divide and conquer by performing parallel spatiotemporal computations. That is, the convergence of large spatiotemporal domains by solving the equations locally on subdomains which communicate with each other after each parallel computation. This type of computation is forbidden by Fourier spectral methods as it assumes periodic boundary conditions. The general case would need to be either finite element or (we believe the better choice) a spectral method which can handle non-periodic boundary conditions such as Chebyshev spectral methods.

7. Future Work.

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- **8. Tiles' GuBuCv17 clippings and notes.** Move good text not used in [17] to this file, for possible reuse later.
- **2016-11-05 Predrag** A theory of turbulence that has done away with *dynamics*? We rest our case.
- 2019-03-19 Predrag Dropped this:

In what follows we shall state results of all calculations either in units of the 'dimensionless system size' \tilde{L} , or the system size $\tilde{L}=2\pi\tilde{L}$.

Due to the hyperviscous damping u_{xxxx} , long time solutions of Kuramoto-Sivashinsky equation are smooth, a_k drop off fast with k, and truncations of (??) to $16 \le N \le 128$ terms yield accurate solutions for system sizes considered here (see Appendix ??).

For the case investigated here, the state space representation dimension $d \sim 10^2$ is set by requiring that the exact invariant solutions that we compute are accurate to $\sim 10^{-5}$.

- **8.1.** GuBuCv17 to do's. Internal discussions of [17] edits.
- 2019-03-17 Predrag to Matt My main problem in writing this up is that I see nothing in the blog that formulates the variational methods that you use, in a mathematically clear and presentable form. Perhaps there is some text from

siminos/gudorf/thesisProposal/proposal.tex

that you can use to start writing up variational justification for your numerical codes, section ?? Variational methods.

- **2019-03-17 Predrag to Matt** Please write up *tile extraction* and *glueing* in the style of a SIADS article.
- 2019-03-17 Predrag to Matt Should any of Appendix ?? Fourier transform normalization factors be incorporated into GuBuCv17 [17]?
- 2019-04-10 Matt writing To begin variational.tex I included two equivalent formulations of the variational problem; the first is written in a more concise manner while the second is written in a more explicit manner. The longer of the two is commented out. The more explicit description uses dummy variables (Lagrange multipliers) which replace parameters (\tilde{L},T) as independent variables.

I'm including explanations of the numerical algorithms but I don't think I should present them in their style for algorithms, because we didn't invent them just applied them in a unique way. If desired I think the easiest way of including them per SIADS style guide is to use the algorithm package they suggest: algpseudocode and algorithmic are the package names.

I feel conflicted as to whether to define the gradient matrix using a new letter or the "mathematician way". e.g. A(x) or DG(x). Also, I started using **z** to represent state space vectors. I'm not a fan of using z but I don't want to confuse people by using u,x, etc.

I need to get better at writing or stop being OCD over how sentences are written.

2019-04-16 Matt update In an effort to make the chapters and GuBuCv17.tex more modular, I've split apart some of the chapters into smaller, more manageable pieces. For example, variational.tex was covering too many topics to be reflected by the file name and numerics.tex predominately covered discrete lagrangian systems and Noether's

theorem. The algorithms (matrix free adjoint descent, matrix free GMRES and Gauss-Newton) have yet to be discussed in excruciating detail. This is my fault, in hindsight I've done a poor job with recording what I do and how I do it. I'm going to get better at this.

For the time being, until it is deemed unnecessary or unintelligent, I am going to break the chapters into the files adjointdescent.tex and iterativemethods.tex. I'm going to change the discourse so that instead of requiring the current order, namely, variational.tex-¿adjointdescent.tex-¿iterativemethods.tex the pieces will be written as to be independent of one another.

In order to get specific, I needed to include the Kuramoto-Sivashinsky equation written in the Fourier-Fourier basis; I put this in sFb.tex

- 2019-04-17 MNG update Realized that in order to get specific with the numerical methods I need to include both an exposition on the spatiotemporal Fourier modes as well as the matrix-free computations. The latter really stresses the improvements over the finite-difference approximation of the Jacobian that requires time integration ubiquitous in plane-couette and pipe numerics. Expanding on adjointdescent.tex and iterativemethods.tex. Again, the main stratagem is to make the separate .tex files as independent as possible to avoid "long distance references".
- 2019-04-18 MNG Heavy edits to tiles.tex Added section on preconditioning preconditioning.tex Formatting edits to matrixfree.tex can be ignored.

Added details in iterativemethods.tex regarding GMRES and SciPy wrapper for LAPACK solver GELSD

2019-04-23 MNG Converting indices to abide by the conventions: physical space indices $u(x_m, t_n)$, and spatiotemporal Fourier space indices $\hat{\mathbf{u}}_{kj}$.

2018-05-09 PC can do. Also, remember that $u(x_m, t_n)$ implies that everywhere the ordering is (\tilde{L}, T) , and not (T, \tilde{L}) .

Luca Dieci asked (borderline pleaded) to abide by the mathematics convention that n is the index for discrete time. I'm avoiding ℓ and τ_t due to the unnecessary confusion with domain size \tilde{L} and period T.

2018-05-09 PC Agreed. τ_t we usually control by macro zeit, so currently t_n .

2019-04-24 MNG Discussion of how I foresee paper(s) playing out in blogMNG.tex by considering subject matter, narratives, and paper length. Perhaps unsurprisingly I lean towards structuring a paper similar to my thesis.

I'm unsure how to approach spatiotemporal symmetries in a practical manner. Projection operators which produces symmetry invariant subspaces are nice and complements the selection rules for different symmetries nicely. Specifically it provides the reason for why the selection rules exist and motivates the use of symmetry constrained Fourier transforms. The only issue I have with this is that the results of the formal derivation are not really used beyong that. I think this is likely a case of "It-is-trivial-now-that-I-know-it' syndrome. Perhaps it would be sufficient to say that the selection rules constitute these subspaces without the formalism?

2019-04-29 MNG Rewrite of KSsymm.tex after double checking the derivations. Going to rewrite sFb.tex, I'm paying for the expedient manner in which is was written; in other words just use a single Fourier basis as opposed to a real basis and a complex basis,

Matt.

2019-04-30 MNG Rewrites to describe the spatiotemporal Kuramoto-Sivashinsky equation only in terms of real valued Fourier coefficients for consistency. The index notation gets a little rough but the pseudospectral form of the equation is nice enough.

Tried to find the most concise description of how I handle relative periodic orbits using mean velocity frame (time dependent rotation transformation).

2019-05-02 MNG Is it necessary to recap all of the results in Sect. ?? in this paper? Other than the spatial integration calculation the results described in [5, 6]. I'm unsure how to connect the spatiotemporal calculations to results pertaining to the dynamical system formulation, e.g. temporal stability and energy budget.

Moved SpatTempSymbDyb.tex to after tiles.tex such that it proceeds from finding tiles to using tiles.

The bulk of each section is complete; perhaps need to add some more detail to glue.tex and tiles.tex but mostly need to work on picking, producing, and inserting figures.

Going to list suggestions for figures at the top of each section in commented text.

2019-05-02 MNG Added tile figures: Extraction and converged results in tiles.tex.

Modifying scripts to produce figures of general numerical convergence (initial condition to final converged doubly-periodic orbit), produce figures demonstrating step-by-step gluing for repeated gluing, and produce figures for the "frankenstein" plots (combining tiles to produce doubly-periodic orbits). Basically just producing more figures.

- 2019-05-11 PC moved Ibragimov to gudorf/thesis/thesis.tex until we find it useful.
- 2019-05-13 MNG
- Added spatial gluing figures
- Added description of gluing procedure
- 2019-05-13 PC Figures are looking great, and in my talks people seem to "get" tile extraction and gluing, so they are very important. A few notes, before you produce the next versions:
 - I think you should label all u color bars in multiples of 1, or or 0.5 if that is really needed, not different units in every plot.
 - Once you have improved a given figure, keep the same name rather than renaming it (they are often shared between different articles, presentations and blogs)
- 2019-07-05 PC dropped from trawl.tex: "In both formulations there is no guarantee of convergence but it is clearly better to take less time regardless of convergence.

In our formulation, convergence can not be guaranteed either, but the resources committed to the initial guesses generation are negligible. "

$$q_{k} = 2\pi \frac{k}{\tilde{L}}, \qquad k = 1, \dots, M/2 - 1$$

$$\omega_{j} = 2\pi \frac{j}{T}, \qquad j = 0, \dots, N/2 - 1$$

$$x_{m} = \frac{m}{M}\tilde{L}, \qquad m = 0, \dots, M - 1$$

$$t_{n} = \frac{n}{N}T, \qquad n = 0, \dots, N - 1.$$

$$(8.1)$$

2019-08-21 MNG Moved discussion of recurrence plots and multiple shooting from trawl.tex to variational.tex

It seemed more coherent to first describe the disadvantages of the IVP to motivate the variational problem. I'm going to refer to what I do as "solving a variational problem" as opposed to boundary value problem because it insinuates (at least to me) that we're solving a Dirichlet BC in 1 + 1 dimensions problem.

General narrative of variational.tex

- Exponential instability bad
- Variational formulation good
- How to solve variational problem (general description of optimization)
- Losses from variational formulation (notion of dynamics, stability, bifurcation analysis).
- How to recoup from these losses (adjoint sensitivity, Lagrangian, Hill's formula) It's currently a hot mess.
- 2019-09-20 MNG Input references to topological defects and motifs in complex networks. Renamed the "defect tile" to the "merger tile" but also made the connection that similar patterns in crystals are referred to as "edge dislocations".

Just clean up and rewriting tiles.tex mainly; it's almost in shape.

2018-05-09 PC Dropped: The following definitions will be devoid of symmetry considerations such that the equations represent the general case.

For $\tilde{L} < 1$ the only equilibrium of the system is the globally attracting constant solution u(x,t)=0, denoted E_0 from now on. With increasing system size \tilde{L} the system undergoes a series of bifurcations. The resulting equilibria and relative equilibria are described in the classical papers of Kevrekidis, Nicolaenko and Scovel [22], and Greene and Kim [16], among others. The relevant bifurcations up to the system size investigated here are summarized in Figure ??: at $\tilde{L}=22/2\pi=3.5014\cdots$, the equilibria are the constant solution E_0 , the equilibrium E_1 called GLMRT by Greene and Kim [26, 16], the 2- and 3-cell states E_2 and E_3 , and the pairs of relative equilibria $TW_{\pm 1}$, $TW_{\pm 2}$. All equilibria are in the antisymmetric subspace \mathbb{U}^+ , while E_2 is also invariant under D_2 and E_3 under D_3 .

Due to the translational invariance of Kuramoto-Sivashinsky equation, they form invariant circles in the full state space. In the \mathbb{U}^+ subspace considered here, they correspond to 2n points, each shifted by $\tilde{L}/2n$. For a sufficiently small \tilde{L} the number of equilibria is small and concentrated on the low wave-number end of the Fourier spectrum.

dropped this: G, the group of actions $g \in G$ on a state space (reflections, translations, etc.) is a spatial symmetry of a given system if $gu_t = F(gu)$.

An instructive example is offered by the dynamics for the $(\tilde{L},T)=(22,T)$ system that [6] specializes to. The size of this small system is ~ 2.5 mean wavelengths $(\tilde{L}/\sqrt{2}=2.4758\ldots)$, and the competition between states with wavenumbers 2 and 3. The two zero Lyapunov exponents are due to the time and space translational symmetries of the Kuramoto-Sivashinsky equation.

For large system size, as the one shown in Figure ??, it is hard to imagine a scenario under which attractive periodic states (as shown in [14], they do exist) would have significantly large immediate basins of attraction.

2019-10-17 MNG: Merged symmetry discussions. KSsymmNG1 was deleted because seems to be an old discussion predating the spatiotemporal symmetry group discussion as it still mentions equivariance. The focus should only be on invariance under symmetry operations, as invariance gives rise to the the practical application of the symemtry discussion which is constraints on the spatiotemporal Fourier coefficients. KSsymmNG was deleted because it is just an older version of KSsymm. KSsymmPC uses different notation and says things better than I do so I'll have to figure out how to merge it in.

2019-10-25 PC dropped from variational.tex:

Linear stability analysis has been used in bifurcation analysis of describe the existence and bifurcations of solutions as well as the geometry of state spaces corresponding to different flows [15, 25, 32].

Commonly time variational integrators preserve symplectic structure

2019-09-05 MNG Dropped from variational.tex: multishooting optimization of cost functional because it doesn't jive with spatiotemporal methods (based on integration) Adjoint sensitivity and Hill's formula sections when I figure them out or they seem useful:

Section on adjoint sensitivity The spatiotemporal reformulation of a dynamical problem also requires a reformulation of its linear stability analysis.

Nevertheless, we still have the notions of tangent spaces and derivatives so the natural replacement is the notion of sensitivity. In the context of finite element (finite difference) representation, instead of computing a derivative and transporting it around a periodic orbit, it instead computes the derivative of the temporal average of the quantity with respect to whichever parameter is desired [1, 27, 34]. Because there is no transport, one need not worry about the exponential instability present. Essentially sensitivity is to stability as boundary value problem is to initial value problem in this context. Because the spatiotemporal boundary problem is defined on a compact domain on which the scalar field does not diverge, dynamical observables are bounded; they do not experience numerical overflow (underflow) associated with unstable (stable) manifolds.

(8.2)
$$S = \int_{\mathcal{M}} \mathcal{L}(u, v, u_x, v_x, u_t, v_t, u_x x, v_x x) dx dt$$

such that the matrix of second variations, or Hessian, of this action functional is

defined as

$$(8.3) H = \nabla \nabla^{\top} S$$

such that the derivatives are taken with respect to the infinite dimensional scalar fields u, v, \ldots , such that the Hessian matrix is infinite dimensional prior to discretization of the scalar fields. The resultant discrete Lagrangian system and subsequent Hessian should be the Hessian of Hill's formula, I believe. If one is trying to derive Hamilton's action principle as a result of discretization (that is, finite differences) as in [23] then one must take care to define spatiotemporal differentiation operators in a manner consistent with an action principle. A large amount of the derivation of the discrete action principle and discrete Noether's theorem of [23] relates to using a finite element discretization in physical space. I am unsure how these ideas extend to a Fourier basis; I currently am assuming that as long as the differentiation operators, and hence the derivatives (jet bundle) is properly defined then everything should work out. When two total derivatives of the Lagrangian density are taken, one arrives at the following matrix representation of the Hessian. Keep in mind that we have ordered the variables in terms of the order of the corresponding derivatives $(u, v, u_t, v_t, u_x, v_x, u_xx, v_xx)$.

$$(8.4) \begin{bmatrix} -v_x(t,x)/3 & u_x(t,x)/3 & 0 & -1/2 & v(t,x)/3 & -2u(t,x)/3 & 0 & 0 \\ u_x(t,x)/3 & 0 & 1/2 & 0 & u/3 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1/2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ v(t,x)/3 & u(t,x)/3 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ -2u(t,x)/3 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

This is an infinite dimensional matrix, but upon discretization each block will represent a diagonal matrix whose diagonal contains the scalar field values of the corresponding spacetime coordinates. For instance, $u_x/3 \equiv \frac{1}{3}u_x(x,t) \to \frac{1}{3}u_x(t_n,x_m)$. Because each of the blocks are diagonal, that is, $1 \equiv \mathcal{I}^{N*M}$, the determinant expansion is long but not impossible to decipher. Note the presence of the adjoint variables v, v_x . There is freedom in the choice of what these variables should be, because they are non-physical. **2020-02-28 MNG** Reformatted the paper into sections which follow the outline so far.

tileoutline.tex, tileintro.tex, tilebody.tex,tilesummary.tex, tilefuture.tex,

Note to Predrag - send this paper to