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A search for the simplest chaotic partial differential equation

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ABSTRACT

A numerical search for the simplest chaotic partial differential equation (PDE) suggests that the Kuramoto–Sivashinsky equation is the simplest chaotic PDE with a quadratic or cubic nonlinearity and periodic boundary conditions. We define the simplicity of an equation, enumerate all autonomous equations with a single quadratic or cubic nonlinearity that are simpler than the Kuramoto–Sivashinsky equation, and then test those equations for chaos, but none appear to be chaotic. However, the search finds several chaotic, ill-posed PDEs; the simplest of these, in the discrete approximation of finitely many, coupled ordinary differential equations (ODEs), is a strikingly simple, chaotic, circulant ODE system.

1. Introduction

The simplest chaotic examples of various types of dynamical systems are instructive because they reveal chaos' universal features and basic ingredients, since distilling complicated chaotic systems down to the simplest one reveals the precious few elements essential for chaos.

For example, the quadratic map

$$x_{n+1} = A - x_n^2 \tag{1}$$

is the simplest chaotic map with a quadratic nonlinearity [1]. (It is chaotic for $A \in (1.4011, \ldots, 2)$, except for infinitely many periodic windows comprising about 10% of the interval.) The "complexity" of an equation requires a definition, to be discussed below, but agreeing that Eq. (1) is the simplest chaotic map is straightforward because it contains the fewest possible terms — just two — and the simplest monomial nonlinearity — x^2. Despite its simplicity, the quadratic map exhibits the general features of more complicated chaotic maps, such as the period-doubling route to chaos.

Similarly, the simplest chaotic flow is $\dddot{x} + A\ddot{x} - \dot{x}^2 + x = 0$ [2], which was found by searching all equations that are simpler than the Lorenz [3] and Rössler [4] systems. It was later proved that no simpler quadratic flows are chaotic [5].

This project performs a similar search for chaos as in [2] but for partial (rather than ordinary) differential equations. Searching for chaos in PDEs, an area not well studied in general, is worthwhile because many of the equations governing the physical universe are nonlinear PDEs (for an extensive list of nonlinear PDEs see [6]).

2. The search

Before embarking on this project, the simplest known chaotic PDE was the Kuramoto–Sivashinsky (KS) equation,

$$u_t = -uu_x - \frac{1}{R}u_{xx} - u_{xxxx}, \tag{2}$$

where $u = u(x,t)$ is a real function of space and time, and R is a constant. (Hereafter we denote partial derivatives by subscripts: for example, $u_t \equiv \partial u/\partial t$, $u_{xx} \equiv \partial^2 u/\partial x^2$, etc.) The KS equation was numerically known to be chaotic for $R = 2$, as illustrated in Fig. 1.

Originally derived to model waves in Belousov–Zhabotinsky reactions [7], the KS equation has found a host of other applications, from flame front modulations [8], to instabilities in cellular flows [13], to flows of thin liquid films (down inclined planes [9], vertical planes [11,12], and vertical columns [10]). This model equation for instabilities in physical systems has been extensively studied analytically (e.g., [14]) and numerically (e.g., [15]).

The astute reader will note that the KS equation is odd (that is, invariant under $x \to -x$, $u \to -u$), but the solution in Fig. 1, which begins with an odd initial condition, violates that symmetry. Chaos

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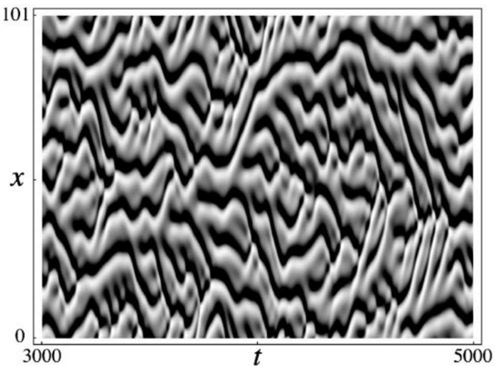

Fig. 1. Chaos is apparent in this density plot of the Kuramoto–Sivashinsky equation, solved here with $R = 2$, 101 coupled ODEs, spatial length $L = 101$, periodic boundary conditions $u(0,t) = u(101,t)$, and initial condition $u(x,0) = 4\sin(2\pi x/101)$. The $u(x,t)$ values are plotted on a grayscale, with darker corresponding to larger $u(x,t)$. The largest Lyapunov exponent, evaluated from time $t = 1.5 \times 10^4$ to 10^5, is 0.028.

is the culprit: a deviation of 10^{-4} from perfect symmetry at time zero (which equals the numerical method's accuracy goal) expands to the size of the system by around time 350, in agreement with numerical experiment.

We searched the space of equations that have the same form as the Kuramoto–Sivashinsky equation. Specifically, we considered explicit, autonomous partial differential equations of the form

$$u_t = F(u, u_x, u_{xx}, u_{xxx}, \ldots), \tag{3}$$

where $F(u(x,t))$ is a polynomial in u and its spatial derivatives, can contain a constant term, and must contain a single nonlinearity that is either quadratic or cubic (e.g., u^2, uu_{xxx}, $(u_x)^3$, etc.). Note that many natural generalizations of the form (3) exist — for example, $u(x,t)$ could be complex- or vector-valued, there could be more than one spatial dimension, or u_t could become u_{tt} or u_{xt}, etc. — but this study searches the space defined by (3) because it is simple yet sufficiently vast.

This study considers periodic boundary conditions, rather than Dirichlet, Neumann or Robin boundary conditions, so the PDEs live on a ring rather than a line segment. Intuitively, periodic boundary conditions seem most likely to permit chaos because they impose the fewest constraints.

The goal was to find equations that are somehow "simpler" than the KS equation yet still chaotic. But first, what is the "complexity" of an equation? There is no universal, accepted definition, so we created our own, which works as follows:

1. Arrange u_t on the left-hand side of the equation and all the other terms on the right-hand side.
2. On the right-hand side, write each power as a product (e.g., write u^2 as uu), and count the number of terms, the number of appearances of u, and the number of appearances of x in subscripts (i.e., the derivatives).
3. The sum of those three quantities is the complexity of the equation.

For example, the term uu_{xxx} would add 6 to the complexity (1 for being a term, 2 for the two u's, 3 for the three x's), while the term $u(u_x)^2 = uu_xu_x$ would add 6 to the complexity (1 for being a term, 3 for the three u's, 2 for the two x's). This definition enjoys many virtues: it is easy to program, easy to state in English, and captures three human notions of the complexity of an equation: adding terms, increasing powers and increasing derivatives all increase the complexity.

Using this procedure, the KS equation has complexity 14. Enumerating all equations with complexity less than 14 and either one quadratic or cubic nonlinearity yields 210 quadratic and 163 cubic equations.

Other definitions of complexity exist, of course, and these could generate different lists of equations that are less complex than the KS equation. However, the equations that would be added to or deleted from the list due to changing the definition of complexity would lie near the boundary between inclusion and exclusion; that is, they would have complexity comparable to that of the KS equation. The majority of the equations in our list — that is, the simplest ones — would appear in most everyone's list of equations less complex than the KS equation.

Twenty-one equations in the list are redundant in the sense that differentiating with respect to x and letting $v \equiv u_x$ yields another equation in the list. However, eliminating these twenty-one equations would not buy much computational savings, and furthermore searching the same equation twice gives more chances to find chaos.

This study searches for spatiotemporal chaos rather than low-dimensional chaos (i.e., purely temporal or purely spatial chaos). The periodic boundary conditions preclude purely spatial chaos, while the lack of second-order or greater time derivatives forbids purely temporal chaos. Furthermore, purely temporal chaos would require no spatial derivatives, which yields only five equations ($u_t = u^2, u^3, 1+u^2, 1+u^3, u+u^3$), all of which are first-order systems and so not chaotic.

To test each equation for chaos, we compute its largest Lyapunov exponent (LLE) [16], the standard test for chaos, which measures the average exponential rate at which nearby initial conditions diverge. If the LLE is positive, then small perturbations grow exponentially in time, predictability is lost, and the system is chaotic.

To calculate the Lyapunov exponent, one repeatedly perturbs the system and computes the separation between the perturbed and unperturbed trajectories. These operations are straightforward for finite systems such as maps and ordinary differential equations because the state variables are scalars and vectors. However, the states of partial differential equations are functions $u(x,t)$, with t fixed and x varying from 0 to the size L of the system. Thus to compute separation distances between functions, we convert the curve $u(x,t)$ into an L-vector by collecting the values at integral positions in space and then proceed with the finite procedure for calculating the Lyapunov exponent as in [17].

The partial differential equations were solved using the built-in numerical differential equation solver in Mathematica 5.2, which uses the method of lines [18]. Though some PDEs are better solved by pseudo-spectral, upwind, or other numerical methods, the formidable scope of this search requires a general-purpose method such as the method of lines, which can efficiently solve a large class of initial value problems.

The periodic boundary conditions imply that $u(0,t) \equiv u(L,t)$ for some fixed L (and the spatial derivatives match at the boundary as well), so one can imagine the PDE as a ring of ODEs — infinitely many of them, each coupled to its nearest neighbors. The numerical method discretizes space using a tensor product grid of at least 101 ODEs, approximates spatial derivatives using fourth-order finite differences, and adapts the temporal step size to satisfy the absolute and relative error goals of 10^{-4} each.

We solve each equation out to time $t = 8000$ (quadratic) or $t = 5000$ (cubic), long enough for solutions converging to a fixed point or to infinity to be easily recognized and discarded. Such methods cut months off the search because they quickly reject non-chaotic equations before laboriously computing their LLE.

We evaluate the LLE from $t = 7000$ to $t = 8000$ (quadratic) or from $t = 4000$ to $t = 5000$ (cubic). Ignoring the first 7000 (quadratic) or 4000 (cubic) time units helps to ensure that the system is on its attractor rather than approaching it, which could give spurious results (transient chaos).

Each candidate equation contains between one and five terms (not counting u_t), each of which is multiplied by a real coefficient. Fortunately, a suitable linear rescaling of u and t normalizes two of the coefficients to ± 1, a trick that significantly reduces the number of possible coefficients. For example, an equation with 3 terms has two coefficients that are ± 1, and the third can be any real number; this third coefficient is like a "knob" that we turn.

The question becomes: what values do you try for the "knobs"? The coefficients should be within a few orders of magnitude of each other, for otherwise the terms with comparatively tiny coefficients hardly affect the system, so they add unnecessary complexity to the equation. Thus we let each coefficient randomly sample hundreds of values in a uniform logarithmic distribution from 10^{-2} to 10^2, and for each value we also try its negative.

The coefficients are not the only parameters to tune: the initial condition $u(x,0)$ can be varied, as well. If an equation is chaotic and dissipative, there exists a "basin of attraction," a region of initial conditions such that the solution is chaotic whenever the initial condition lies in its basin of attraction. Therefore, if a candidate equation is chaotic, the computer search must test that equation using an initial condition in its basin of attraction. Like fishermen casting a large net, we try dozens of initial conditions, hoping at least one lies in the basin of attraction (provided it exists). (Note that conservative systems have no basin of attraction but instead a "chaotic sea," although the idea is the same, except that there are no transients.) In particular, we tried initial conditions of the form

$$u(x,0) = A\sin\left(\frac{2\pi}{P}\frac{x}{L}\right) + V, \tag{4}$$

where L is the circumference of the ring (we tried all primes between $L = 2$ and $L = 29$), P is the period (we tried $P = \frac{1}{2}$, 1, 2), V is the vertical offset (we tried 7 roughly evenly spaced values between -1 and 1, including 0), and the amplitude A is fixed at 1. Note that initial conditions with $P = 2$ have a discontinuous derivative at $x = 0$, a virtue since it expands the types of initial conditions used in the search. The exact form of the initial condition is not too important since the system eventually finds its attractor provided that the initial condition lies in the basin of attraction (if the equation is dissipative) or chaotic sea (if the equation is conservative).

3. Results of the search

We ran this search on a 2 GHz dual-core CPU for 16 months, trying thousands of coefficients and initial conditions for each of the 373 candidate equations, yet we found no chaotic solutions. Furthermore, the search successfully detects chaos — testing the KS equation with spatial length $L = 19$ finds 80 chaotic solutions — so it is unlikely any of the candidate equations are chaotic.

The following examples illustrate the behavior of the 373 equations in the search.

Example 1. The equation

$$u_t = \pm u \pm u^3 + c u_{xxx} \tag{5}$$

typifies the behavior of 90% of the 373 equations in the search. The solutions either

- decay to the attracting "fixed point" $u \equiv 0$,
- diverge to infinity,
- or are periodic (i.e., a traveling wave)

in approximately a 2:1:1 ratio. The behavior of Eq. (5) depends on the signs of the first two terms. If the sign of u is negative, then the system is damped and decays to $u \equiv 0$ because there is no energy input. On the other hand, if the signs are $+u + u^3$, nothing damps the energy input, so solutions diverge to infinity, whereas the signs $+u - u^3$ lead to a traveling wave with velocity and shape determined by the constant c (see Fig. 2). The search method quickly detects behavior of the first two types, and the calculated largest Lyapunov exponent for the third type is zero.

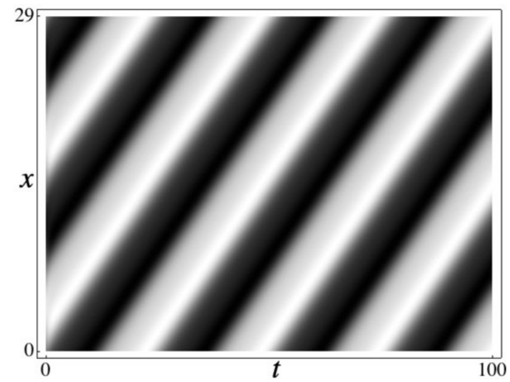

Fig. 2. Traveling wave behavior of $u_t = u - u^3 + u_{xxx}$

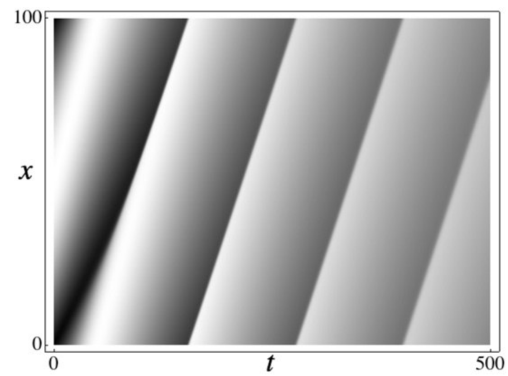

Fig. 3. Shocks, or waves with steep wavefronts, quickly form in the solution to Burgers' equation, which is not chaotic.

Example 2. Whereas Eq. (5) can diverge to infinity because the energy increases without bound, other equations diverge to infinity because singularities form in the derivative u_x. For example, Burgers' equation [19]

$$u_t = \pm u_{xx} \pm u u_x \tag{6}$$

is an integrable system that exhibits shocks, propagating waves with steep wavefronts, as shown in Fig. 3. About 8% of the 373 equations in the search exhibited behavior of this type, and sometimes the wavefront becomes so steep that u_x becomes unbounded. The search method quickly recognizes and discards equations that form such singularities.

Example 3. The remaining 2% of the candidate equations are the most interesting and exhibit behavior similar to that of the system

$$u_t = (u_x)^3, \tag{7}$$

which is a chaotic PDE with a complexity of 7 (half that of the KS equation). Unfortunately, Eq. (7) is ill-posed, as explained below. Not surprisingly, equations with a similar form as Eq. (7) — namely, a product of three odd-degree derivatives (of which there are six: $(u_x)^3$, $(u_x)^2 u_{xxx}$, $u_x(u_{xxx})^2$, $u_x u_{xxx} u_{xxxxx}$, $(u_x)^2 u_{xxxxx}$, $(u_x)^2 u_{xxxxxxx}$) — all appear to be chaotic but ill-posed like (7).

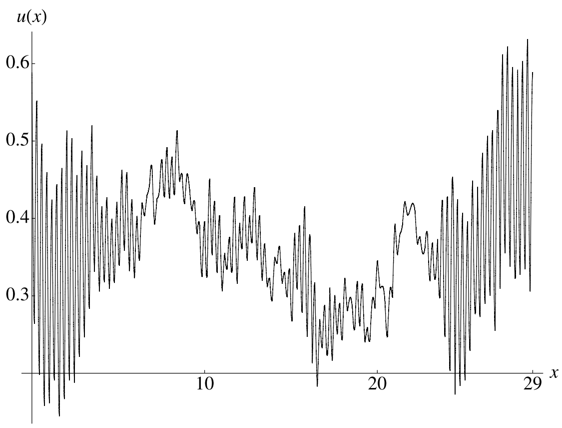

Fig. 4. Short wavelength behavior at the level of the spatial discretization is apparent in the solution of $u_t = (u_x)^3$ at time $t = 10\,000$, approximated here using 201 ODEs.

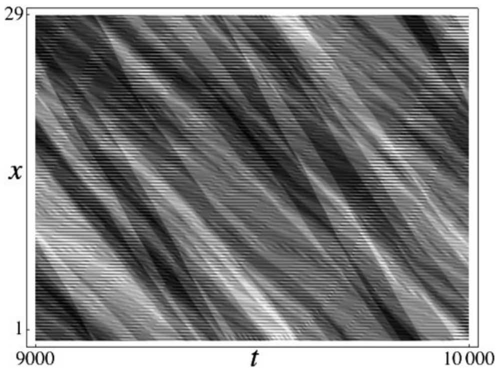

Fig. 5. A density plot of $u_t = (u_x)^3$ solved with 201 ODEs shows the short wavelength behavior at the level of the spatial discretization, which appear as parallel, horizontal bands resembling corduroy.

Eq. (7) is ill-posed because the energy cascades to the shortest wavelength equal to twice the spacing used by the numerical method. That is, if the numerical method approximates the PDE as N coupled ODEs, and the spatial length of the system is L, then the shortest possible wavelength is $2L/N$ — precisely the wavelength at which energy accumulates. As shown in Fig. 4, the solution oscillates between high and low values at successive spatial locations. This pathological behavior is also apparent in the density plot in Fig. 5, where the short wavelength behavior at the size of the spatial discretization looks like corduroy superimposed on diagonal striations.

Crucially, in the PDE limit of increasing fineness of the spatial grid, the energy goes to shorter wavelengths *in lockstep with the spatial grid* because there is no hyperviscosity term (such as $-u_{xxxx}$ in the KS equation) to damp short wavelengths. To quantify this relationship, we examined Eq. (7) as a system of N coupled ODEs $u_1(t), \dots, u_N(t)$ evolving with periodic boundary condition according to

$$\frac{du_i}{dt} = \gamma (u_{i+1} - u_{i-1})^3, \tag{8}$$

where $\gamma \equiv (N/2L)^3$. To see why Eq. (8) approximates the PDE (7), observe that for N ODEs on a ring of length L, the spacing is L/N, so the first spatial derivative is approximately

$$\frac{du_i}{dx} \approx \frac{u_{i+1} - u_{i-1}}{2L/N},$$

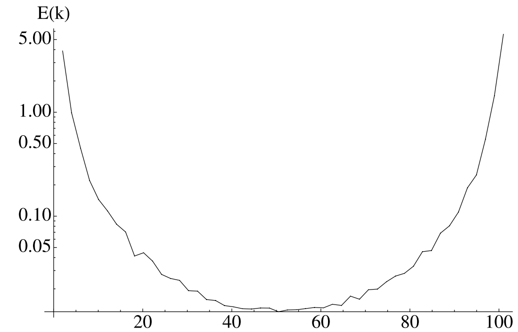

Fig. 6. The energy $E(k)$ as a function of the wavenumber $k \equiv 202/\lambda$ for the ill-behaved coupled ODE system (8) illustrates the energy piling up at the shortest wavelengths (highest k). This curve is the square of the modulus of the discrete sine Fourier transform of the solution to Eq. (8), averaged from time 3000 to 5000, and connected by lines.

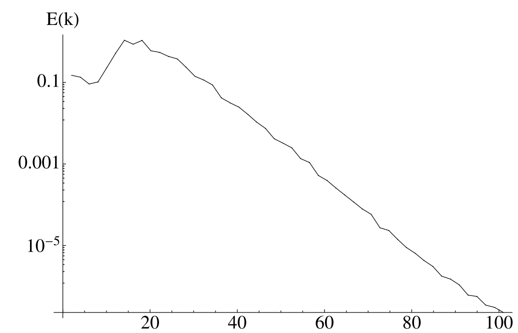

Fig. 7. The spectral density for the discrete approximation of the Kuramoto–Sivashinsky equation shows why it is well-behaved: the energy is concentrated at long and intermediate wavelengths and thereafter decays exponentially with increasing wavenumber (decreasing wavelength). This curve is computed in the same way as in Fig. 6.

the cube of which is the right-hand side of (8). Therefore, to examine how Eq. (7) misbehaves as a PDE, we explore how its discrete approximation (8) depends on the spatial step size $\Delta x \equiv L/N$ by varying the coefficient γ.

The spectral density of the solution to Eq. (8) confirms our intuition that the energy piles up in the shortest wavelength (highest wavenumber $k \equiv 202/\lambda$). As shown in Fig. 6, the energy is concentrated at the shortest and longest wavelengths and scarce at intermediate wavelengths. Contrast this with the corresponding plot for the KS equation in Fig. 7; for this well-behaved equation the energy is concentrated at intermediate wavelengths and negligible at the smallest wavelength.

In addition to the energy cascading to the shortest wavelength, the largest Lyapunov exponent of the coupled ODE system (8) also indicates why its PDE limit (7) is ill-behaved. By dimensional analysis, the LLE is proportional to $A^2\gamma$, where A is the amplitude of the initial condition. Experimental verification of LLE $\propto \gamma$ is shown in Fig. 8, and we have similarly verified the proportionality with A^2.

That the LLE and γ are proportional suggests the LLE becomes infinite in the PDE limit of infinite γ. Although linearly rescaling t or u appears to resolve this issue by making the LLE finite and well-defined, such a rescaling leads to more issues, further evidence that Eq. (7) is pathological. For instance, rescaling time according to $\tau \equiv \gamma t$ eliminates γ from the right-hand side of Eq. (8), but now the dynamics occur γ times more quickly. Thus the energy piles up at the shortest wavelengths in space *and in time*. Alternatively, one could linearly rescale u according to $v \equiv u\sqrt{\gamma}$, or equivalently reduce A by $\sqrt{\gamma}$; but this implies that for the

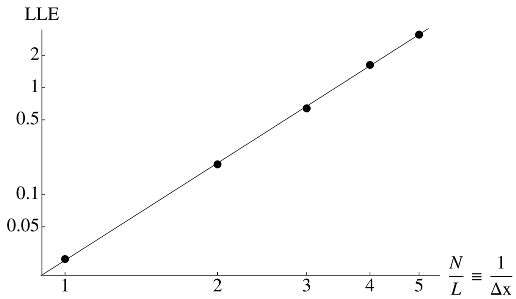

Fig. 8. The largest Lyapunov exponent increases as $0.024(N/L)^{3.02}$, consistent with the expectation that the relationship is cubic. Here we solved Eq. (8) using $N = 101$ ODEs, fixed the amplitude A of the initial condition at 4, and evaluated the LLE from time 10^5 to 1.5×10^5.

PDE (7) to have a well-defined LLE the initial condition must be identically zero. Thus no matter how γ is eliminated by rescaling t or u, the coupled ODE system is ill-behaved in the PDE limit.

The equation $u_t = (u_x)^3$ along with the five other equations mentioned above all appear to exhibit the same behavior: they are chaotic but suffer from pathological behavior at the shortest wavelengths, and no rescaling appears to salvage them.

4. Conclusion

The results of this computer search suggest that the Kuramoto–Sivashinsky equation is the simplest chaotic autonomous PDE with a single quadratic or cubic nonlinearity. However, this result is not definitive: an equation could have a tiny window of coefficients and region of initial conditions that yield chaos. In fact, finding chaos in conservative systems is especially difficult because chaotic seas (the regions of initial conditions that yield chaotic solutions) can be tiny. However, the basins of attraction of dissipative systems are usually large. Since 322 of the 373 candidate equations (86%) are dissipative, this null result has a high degree of certainty for nearly all of the equations.

The fact that no simpler equations were found to be chaotic has implications for the KS equation. Each of its terms, for example, is vital for chaos: energy enters the system at long wavelength via u_{xx}, cascades to short wavelength due to the nonlinearity uu_x, and dissipates via u_{xxxx}. The absence of any of these three terms eliminates the perpetual, aperiodic movement of energy around the system.

Furthermore, simplifying terms in the KS equation eliminates the chaos. It is tempting, for instance, to replace the dissipation $-u_{xxxx}$ with a simpler dissipation such as $-u$, but such a simplification destroys the chaos.

Acknowledgements

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