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We propose the following model equation, $u_t + 1/2(u^2 - uu_s)_x = f(x, u_s)$ that predicts chaotic shock waves, similar to those in detonations in chemically reacting mixtures. The equation is given on the half line, $x < 0$, and the shock is located at $x = 0$ for any $t \geq 0$. Here, $u_s(t)$ is the shock state and the source term f is taken to mimic the chemical energy release in detonations. This equation retains the essential physics needed to reproduce many properties of detonations in gaseous reactive mixtures: steady traveling wave solutions, instability of such solutions, and the onset of chaos. Our model is the first (to our knowledge) to describe chaos in shock waves by a scalar first-order partial differential equation. The chaos arises in the equation thanks to an interplay between the nonlinearity of the inviscid Burgers equation and a novel forcing term that is nonlocal in nature and has deep physical roots in reactive Euler equations.

Shock waves arise in a wide range of physical phenomena: gas dynamics, shallow water flows, supernovae, stellar winds, traffic flows, quantum fluids, and many others [1–3]. The theory of shock waves has a rich history beginning with the fundamental contributions by Riemann in the mid-19th century. Nevertheless, due to the complexity of the underlying governing equations, many open questions remain, especially in problems involving dynamical interactions of shock waves with magnetic and gravitational fields, chemical reactions, and radiation.

Our focus in this Letter is on a fascinating feature of shock wave propagation in chemically reacting media: *shock wave chaos*, in which the shock speed oscillates chaotically. This phenomenon occurs in gaseous detonations as seen in numerical simulations of reactive Euler equations [4,5]. In detonations, a shock wave propagates in a combustible medium (for example, a gaseous mixture of hydrogen and air), ignites the medium, and is sustained by the energy released in the burning mixture. During the chemical reaction, the mixture temperature rapidly rises and, because the gas expansion is slow, the resulting pressure buildup gives rise to strong compression waves. These waves can reach the shock because the flow immediately behind the shock is subsonic. The detonation-shock propagation is sustained by those pressure waves in the reaction zone that reach the shock.

The classical model of detonation, pioneered by Zel'dovich, von Neumann, and Döring (ZND model, [2,6]), is based on a system of reactive Euler equations in one dimension, that consists of equations for the balance of mass, momentum, energy, and the fuel concentration. This system describes four families of waves: one acoustic and two material-entropic waves that propagate away from the

shock, and one acoustic wave that propagates toward the shock. These waves interact nonlinearly with each other and with the shock and can amplify due to the chemical energy release. It is these interactions that are responsible for the detonation-wave dynamics, wherein the shock oscillates in a periodic or chaotic fashion [5]. The main questions in understanding the physical mechanism of these oscillations are: How does this wave amplification occur, and which wave interactions are responsible for the chaos? Do all four families of waves in the reactive Euler equations have to be accounted for or is there a simpler mechanism?

These difficult questions are still largely open. However, the model that we propose here suggests that the mechanism is in fact rather simple. We show that the complex dynamics of one-dimensional detonations are captured by considering only two wave families: very fast waves reflecting off the shock into the reaction zone and slow waves moving from the reaction zone toward the shock; moreover, the fast waves can be assumed to be infinitely fast [7]—the model still retains all the essential features. The infinite-speed assumption leads to a single equation of a very unusual type: a nonlocal first-order hyperbolic partial differential equation. Its solutions provide a strong indication that there exists a simple mechanism hidden in the Euler equations that is responsible for the complex behavior of reactive shocks in gas dynamics.

Before introducing our model, we recall that Burgers [8] proposed his equation, $u_t + uu_x = \epsilon u_{xx}$ (subscripts t and x indicate partial derivatives and $\epsilon \geq 0$ is a viscosity coefficient) in the hope of capturing the essential nature of turbulence with a simple and tractable model. Following a similar idea, Fickett [9,10] and Majda [11] introduced

simple analog models for detonations in the hope of gaining some insight into their behavior. Fickett's model is a modification of the Burgers' equation and takes the form:

$$ut + \frac{1}{2}(u^2 + q\lambda)_x = 0, \qquad \lambda_t = \omega(\lambda, u), \qquad (1)$$

where u is the primary unknown mimicking density, temperature, or pressure, ω is a given chemical rate function, and $q > 0$ is a constant measuring the total chemical energy release (i.e., $q\lambda$ is a fraction of energy released at any given time). The chemistry here is represented by the reaction reactants $\rightarrow$ products, with λ measuring a normalized concentration of the reaction products; it varies from $\lambda = 0$ at the shock to $\lambda = 1$ in the products. Even though Fickett's model has been shown to reproduce some of the features of detonations [9,10,12], the key unstable character of detonations was not seen in this model until Radulescu and Tang [13] extended it to a two-step chemical reaction with an inert induction zone followed by an energy-releasing reaction zone.

To underscore the physical origins of our model, we show now that it is closely related to the theory of Rosales and Majda [14], which is (in contrast to the *ad hoc* models of Fickett and Majda) based on weakly nonlinear asymptotic approximations of the Euler equations. In Ref. [14], the following reduced system for the evolution of detonations was derived:

$$u_\tau + \frac{1}{2}(u^2)_\xi = q\lambda_\xi, \qquad \lambda_\xi = \omega(\lambda, u), \qquad (2)$$

where τ and ξ are time and space, respectively, and u is a temperaturelike variable. The reaction rate ω was chosen to be of the ignition-temperature type with $\omega > 0$ if $u > 0$ and $\omega = 0$ if $u < 0$. The validity of the model derivation is, however, not restricted to this type of rate function. The key difference between the Fickett-Majda models and Eq. (2) is that the rate equation in Eq. (2) involves the space derivative as opposed to the time derivative in Eq. (1). Physically, this means that in Eq. (1), the rate equation does not propagate any waves, while in Eq. (2), waves are propagated instantaneously by the second equation.

For Eq. (2), consider a shock at $\xi = \xi_s(\tau)$, moving into a uniform state ahead of the shock, where $u = 0$ and where there is no reaction, $\omega = 0$. Assume that the reaction is triggered by the shock, and it is such that at $\xi < \xi_s$, ω depends only on the shock state, $u_s = u_s(\tau) =$ the value of u immediately behind the shock, i.e., $\omega = \omega(\lambda, u_s)$. This assumption is sometimes made in modeling condensed-phase explosives [10]. The idea is that the reaction rate is mostly determined by how hard the shock hits a fluid element. Then, the rate equation in Eq. (2) can be integrated to yield λ as a function of ξ and u_s. Hence, the first equation in Eq. (2) takes the form

$$u_\tau + \frac{1}{2}(u^2)_\xi = f(\xi - \xi_s, u_s), \qquad (3)$$

where $f = q\lambda_\xi$ vanishes for $\xi > \xi_s$. The shock speed, $V = d\xi/d\tau$, follows from the Rankine-Hugoniot shock condition [1], $-V[u] + \frac{1}{2}[u^2] = 0$, where the brackets $[*]$ denote the jump of the enclosed quantity across the shock (the value behind minus the value ahead). Since $[u] = u_s$ and $[u^2] = u_s^2$, it follows that $V = u_s/2$.

Next, we change coordinates to the shock-fixed frame, introducing $x = \xi - \xi_s(t)$ and $t = \tau$. Then, Eq. (3) yields the following nonlocal partial differential equation:

$$u_t + \frac{1}{2}(u^2 - uu_s)_x = f(x, u_s), \qquad (4)$$

which must be solved in $x \leq 0$ and $t \geq 0$. Here, $u_s(t) = u(0, t)$, the boundary value of the solution, is not prescribed *a priori*, but follows by solving Eq. (4), as explained below. The function f is chosen such that it mimics the typical behavior of the reaction rate in reactive Euler equations, with a maximum some distance away from the shock (see, e.g., Ref. [2], p. 47). The location of this maximum is chosen to depend sensitively on the shock—state a common feature in the reactive Euler equations, where the reaction rate depends exponentially on the temperature as $\omega \sim \exp(-E/RT)$, with E the activation energy and R the universal gas constant.

Equation (4) is thus a model for the reaction zone of a detonation in coordinates attached to the leading shock. By construction, this shock is located at $x = 0$ at any time. We also assume that the shock satisfies the usual Lax entropy conditions [15], such that the characteristics from both sides of the shock converge on the shock. In characteristic form, Eq. (4) is written as $du/dt = f(x, u_s)$ along $dx/dt = u - u_s/2$. Assuming that $u = 0$ ahead of the shock, it follows that $u_s > 0$ guarantees the Lax conditions. Importantly, no boundary condition at $x = 0$ is needed, as the characteristics from $x < 0$ are outgoing, i.e., $dx/dt|_{x=0-} = (u - u_s/2)_{x=0-} = u_s/2 > 0$. Note that u_s measures the shock strength, because $u_s = [u]$.

The most unusual mathematical feature of Eq. (4) is that it contains the boundary value of the unknown, $u_s(t)$. This is in fact the main reason for the observed complexity of the solutions and has a simple physical interpretation: the boundary information from $x = 0$ is propagated *instantaneously* throughout the solution domain, $x < 0$, while there is a finite-speed influence propagating from the reaction zone back toward the shock along the characteristics of Eq. (4). In the Euler equations, this situation occurs in a weakly nonlinear reactive shock wave, where the flow behind the shock is nearly sonic relative to the shock [14]. One family of acoustic characteristics is then nearly parallel to the shock, representing the slow part of the wave moving toward the shock. The other waves move away from the shock and comprise the influence of the shock on the whole postshock flow. This occurs on a much faster time scale than the information flow toward the shock. At leading order, in the limit considered in Ref. [14], this yields an instantaneous effect.

Returning to the analysis of Eq. (4), we can easily obtain its steady-state solution, $u_0(x)$, by solving

$$\frac{1}{2}(u_0^2 - u_0 u_{0s})' = f(x, u_{0s}), \quad (5)$$

where the prime denotes the derivative with respect to x and the subscript 0 denotes the steady state. The solution is $u_0(x) = u_{0s}/2 + \sqrt{u_{0s}^2/4 + 2\int_0^x f(y, u_{0s})dy}$. The choice of the steady-state shock strength, $u_{0s} = 2\sqrt{2\int_{-\infty}^0 f(y, u_{0s})dy}$, corresponds to the Chapman-Jouguet case in detonation theory [2], since then the characteristic speed at $x = -\infty$ is $u_0(-\infty) - u_{0s}/2 = 0$, indicating that the sonic point is reached at $x = -\infty$. The steady solution can now be written as

$$u_0(x) = \frac{u_{0s}}{2} + \sqrt{2\int_{-\infty}^x f(y, u_{0s})dy}. \quad (6)$$

Clearly, for $u_0(x)$ to be real and bounded, we must require that $0 \leq \int_{-\infty}^x f(y, u_{0s})dy < \infty$ for any $x \in (-\infty, 0]$. This constraint means that the source term must have finite energy and must be positive overall in order for the solutions to make sense. Physically, this also means that the energy must be released rather than consumed to sustain the shock.

Now, we explore the fully nonlinear and unsteady solutions of Eq. (4) for the particular case when

$$f = \frac{q}{2} \frac{1}{\sqrt{4\pi\beta}} \exp\left[-\frac{[x - x_f(u_s)]^2}{4\beta}\right]. \quad (7)$$

We choose $x_f = -k(u_{0s}/u_s)^\alpha$ to make the position of the peak of f to be a sensitive function of u_s; here, $q > 0$, $k > 0$, $\alpha \geq 0$, and $\beta > 0$ are parameters. Next, we rescale the variables as follows: u by u_{0s}, so that the dimensionless steady-state shock strength is 1, length by $l = k$, and time by $\tau = l/u_{0s}$. From Eq. (6), putting all the dimensionless variables in and rescaling β by l^2, we obtain (keeping the same notation for the dimensionless variables and parameters)

$$u_0(x) = \frac{1}{2}\left[1 + \sqrt{\frac{1 + \mathrm{erf}((x + 1)/2\sqrt{\beta})}{1 + \mathrm{erf}(1/2\sqrt{\beta})}}\right], \quad (8)$$

where $\mathrm{erf}(x)$ is the error function. The dimensionless form of Eq. (4) is

$$u_t + \frac{1}{2}(u^2 - uu_s)_x = a \exp\left[-\frac{(x + u_s^{-\alpha})^2}{4\beta}\right], \quad (9)$$

where $a = 1/[4\sqrt{4\pi\beta}(1 + \mathrm{erf}(1/2\sqrt{\beta}))]$. Equation (9) now contains only two parameters: α, reflecting the shock-state sensitivity of the source function, f (an analog of the activation energy in detonations), and β, reflecting the width of f (an analog of the ratio between the reaction-zone length and the induction-zone length).
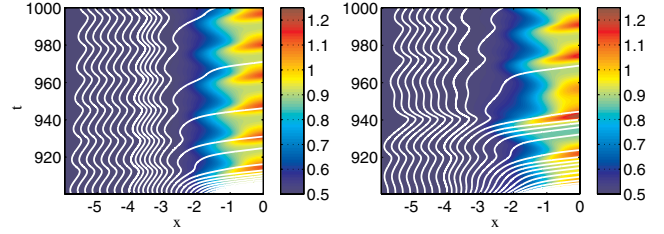

FIG. 1 (color online). The long-time spatiotemporal profiles of $u(x, t)$ (color) for the periodic solution at $\alpha = 4.7$ (left) and the chaotic solution at $\alpha = 5.1$ (right); $\beta = 0.1$. The white curves are the characteristics of Eq. (9) given by $\dot{x} = u - u_s/2$. At any fixed t, $u(x, t)$ generally decreases away from $x = 0$.

In the computations below, we use the numerical algorithm of Ref. [4], which is fifth order accurate in space and third order accurate in time. Our domain has length 10 with 3000 uniformly spaced grid points on it. We find this domain to be sufficiently large for the present calculations, but larger domains may be required for other parameters. We note, however, that due to the rapid decay of $f(x, u_s)$ as $x \to -\infty$, all the dynamics of the solutions are localized in the region close to the shock, $x = 0$. This is shown in Fig. 1, wherein the characteristics are seen to be almost vertical (on average) far from the shock, indicating that the far-field influence on the shock dynamics rapidly diminishes with the distance from the shock. The precise nature of the solutions shown in Fig. 1 (periodic at $\alpha = 4.7$ and chaotic at $\alpha = 5.1$) is confirmed in Fig. 2 (left) for the limit cycle at $\alpha = 4.7$ and Figs. 3–5 for the chaotic solution at $\alpha = 5.1$.

We fix $\beta = 0.1$ and vary α in all the calculations. Our simulations start with the steady-state solution perturbed by numerical noise. Below the critical value $\alpha_c \approx 4.04$, the solution is found to be stable. This critical value is also in agreement with a linear stability analysis of the problem (to be reported elsewhere). At $\alpha = \alpha_c$, a Hopf bifurcation occurs and a limit cycle is born (the shock strength u_s oscillates periodically in time). As α is increased from $\alpha_1 = 4.70$ to $\alpha = 4.85$, a period doubling occurs, see Fig. 2. Remarkably, as α is increased further, we observe
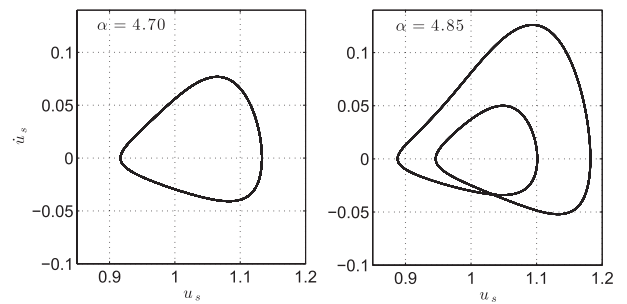

FIG. 2. The period-one and period-two limit cycles in the plane of the shock strength $u_s(t)$ vs $\dot{u}_s$ at two different values of α and $\beta = 0.1$.
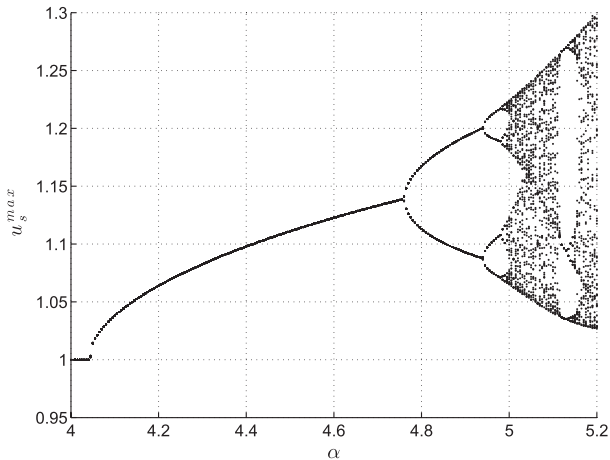
FIG. 3.   The long-time values of the local maxima, $u_s^{\max}$, of the shock strength as a function of α.

a sequence of period-doubling bifurcations that leads to chaotic solutions at α that are slightly larger than 5, as seen in Fig. 3. The onset of chaos apparently follows the same scenario as in the logistic map [16,17]. The bifurcation diagram in Fig. 3 was computed by solving Eq. (9) until $t = 6000$ for the range of α from 3.9 to 5.2, with an increment of 0.005. For each α, we found the maxima of $u_s(t)$ between $t = 5000$ and $t = 6000$ and plotted them in the figure. Based on a sequence of three period doublings, we estimated the Feigenbaum constant, δ [18], to be about 4.5. This is in rough agreement with the well-known value of $\delta = 4.669\ldots$ for the logistic map, as well as that found for detonations [4,5,13,17]. Figure 4 shows the chaotic attractor at $\alpha = 5.1$, in the $(u_s, \dot{u}_s, \ddot{u}_s)$ space (the dots indicate the time derivatives). Its resemblance to the Rössler attractor [19] is evident. Interestingly, when plotting the local maxima of u_s versus their prior values (i.e., the Lorenz map
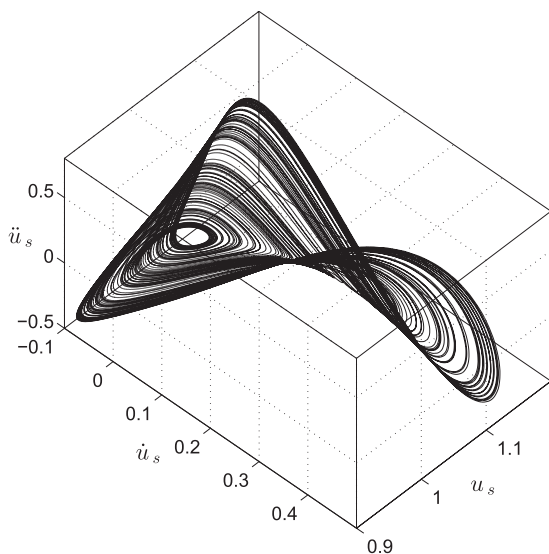
[20], see Fig. 5, the data fall (almost) on a curve. The curve also resembles the one for the Rössler attractor. These observations suggest that the shock wave chaos arising from Eq. (4) is controlled by a low-dimensional process similar to that of a simple one-dimensional map—just as it is the case with the Lorenz and Rössler attractors [17].

The present model and Ref. [13] provide examples demonstrating that the models of Fickett [9] and Majda [11] and the theory of Rosales and Majda [14] do, in fact, contain the complicated instabilities that they were introduced to capture. Here and in Ref. [13], the underlying physics of the detonation phenomenon are faithfully represented, which is the main reason for the observed rich dynamics. Our results contrast a long-held belief that such simplified models may not possess the necessary complexity and may only exhibit stable shocks (see Ref. [21] and references therein for related mathematical results). Stability is indeed the case when the reaction rates lack sufficient sensitivity to the shock state. However, once such sensitivity is present and the feedback mechanism between the shock and the reaction zone is true to the physics of detonation, these simplified models do possess intricate dynamics akin to that of real detonations.

The difficulty of obtaining a reduced theory of detonation has even led to speculating an (admittedly "overpessimistic") possibility that "the phenomenon of detonation structures belongs to the "no theory" category because it might not be reducible to less than the compressible reactive Euler equations" (Ref. [22], p. 665). Our model is strong evidence that this is not so. Detonation can be described by theories that are simpler than the reactive Euler equations; in fact, they can be as simple as one scalar equation. We hope that future research in this direction will further demonstrate the richness and relevance of such simplified models, especially going beyond the simplest one-dimensional model introduced in this work, toward many complex problems in detonation and shock wave physics.
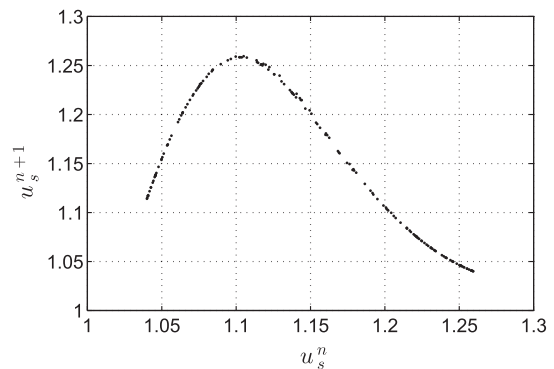

FIG. 4.   The chaotic attractor in the $(u_s, \dot{u}_s, \ddot{u}_s)$ space; $\alpha = 5.1$.

FIG. 5.   The Lorenz map showing consecutive local maxima (u_s^n, u_s^{n+1}) of the shock strength, $u_s(t)$, over large times (from $t = 3000$ to $t = 6000$) for the chaotic case at $\alpha = 5.1$.

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