Evidence for self-organized criticality (SOC) in the non-linear dynamics of detonations

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Abstract

We study the non-linear dynamics of galloping unstable detonations, characterized by a complex sequence of initiation and failure. We analyze the time-series of the lead shock obtained numerically over very long periods. Calculations are reported for the reactive Euler equations and the reduced Fickett reactive Burgers equation model. The detonation speed dynamics develop an approximate self-similar power law scaling, with a power spectrum scaling like $1/f$ over at least one decade of scales. This is characteristic of Self-Organized Criticality (SOC), i.e., the scale-free organization of the dynamics on large scales with no characteristic time, shared by many systems in nature governed by avalanche-like dynamics for energy release (e.g., earthquakes, evolution, sand-pile avalanches, droplet coalescence). We argue that detonations offer a unique deterministic paradigm to study SOC in avalanche dynamics and inverse energy cascades. We discuss the organization of the detonation front dynamics in terms of the physics controlling the wave front evolution. It is found that the largest ”avalanches” trigger the longest lived shock relaxation by the gasdynamic relaxation, involving the expansion wave catching up to the front. Instability in the decaying front triggers a hierarchy of smaller avalanches superposed on the larger ones in a fractal-like structure. These dynamics are discussed in the context of our earlier high order non-linear oscillator model (Bellerive, ICDERS 2016).

1 Introduction

Bak, Tang and Wiesenfeld’s celebrated 1987 *Physical Review Letters* paper first suggested a unique universality class for many complex systems in nature [1]; see [2–4] for recent reviews. Their paradigm attempted to provide a dynamic explanation for the fractal, scale-free nature of many natural phenomena: systems which evolve through a scale-free sequence of cascades, intermittent bursts releasing slowly-accumulated stored energy after certain delay times. A unique feature of this so-called *Self-Organized Criticality* (SOC) is the absence of a characteristic time scale in the dynamics. The frequency of the releasing events are then expected to scale as a power law with respect to their magnitude. A classic example is the earthquake distribution law, whereby the frequency of earthquakes scales with the inverse of their magnitude. Avalanches on a sand pile also capture the same physics: stresses are relieved by avalanches and the magnitude of the avalanche depends on the sequence of previous avalanches or releases, that have each released part of the accumulated stresses. These systems dynamically self-organize to achieve SOC without any external tuning parameter. Examples of SOC and the corresponding $1/f$ scaling have also been suggested in many branches of physics and biology. For example,

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evolution of species is believed to evolve by punctual events. Recent work suggests that human consciousness, characterized by the ability of the human mind to generate transcendental thoughts, may also obey SOC, a feature of real intelligence [5]. In spite of the excitement driven by these discoveries, a formalism for SOC is still lacking. While the dynamics of complex systems do appear to evolve towards SOC, SOC is believed to be an emergent phenomenon. Simple cellular automata models have been shown to obey SOC, but their connection to the underlying physics is not very clear.

Detonation waves, particularly very unstable ones, have in principle the desired physics to display SOC. The instability mechanism is due to the coupling between the forward facing waves and induced exothermicity by the lead shock compression [6]. For galloping detonations, the system evolves through a sequence of detonation failures, where non-reacted gas accumulates behind the lead shock, and re-ignitions [7]. Upon re-ignition, fast flames propagate in the shocked gases and amplify the lead shock upon arrival at the front. The magnitude of the "kick" depends on the amount of gas that has gone unreacted. In this sense, a detonation is essentially an energy accumulation and release complex, similar to sand-piles, earthquakes and many other non-linear systems characterized by energy storage and release.

Qualitatively, it has been shown that one-dimensional detonation dynamics enter a regime of chaotic pulsations for sufficiently sensitive detonations [8–10]. Direct simulation have indeed shown that the front dynamics undergo a sequence of period-doubling bifurcations before acquiring a very irregular pattern of oscillation. This sub-harmonic bifurcation process was shown to persist in the non-periodic regime, with the organization of the front dynamics in lower frequencies. The state of the art is summarized by Powers [11]. The sub-harmonic energy transfer was shown to be universal for many detonation models based on the reactive Euler and Navier Stokes equations [10] and for much simpler toy models based on the Fickett-Majda type of a reactive inviscid Burgers equation with a a forcing responding exponentially to the shock state [6, 12].

In the present study, we test quantitatively whether the dynamics of pulsating detonations in 1D do display SOC in the limit of high instability . We thus conduct long time simulations of unstable detonations of both the reactive Euler and Fickett detonation models and analyze their non-linear dynamics, testing for the characteristic $1/f$ scaling.

2 SOC in the Euler detonation model

We first report on calculations of the reactive Euler equations with a single step Arrhenius reaction. Scales for non-dimensionalization use the initial gas pressure $\hat{p}_0$, density $\hat{\rho}_0$ and the half reaction length of the steady ZND detonation $\hat{\Delta}_{1/2}$. We take the standard non-dimensional heat release $Q = 50$ and isentropic exponent $\gamma = 1.2$ and vary the activation energy Ea. For reference, the neutral stability occurs at $E_a = 25.3$, while period doubling bifurcations persist until $E_a = 27.8$, for larger activation energies, very irregular pulsations are generally observed, with internal shocks being developed at approximately $E_a = 28.8$ [8, 9].

The calculations are performed in a shock-attached frame by a technique described elsewhere [13]. The solution was obtained on a uniform grid of 128 points per ZND half reaction zone length, extending 1000 half reaction zone lengths. The very large domain is required to ensure a negligible influence of the rear boundary conditions on the dynamics. For initial conditions, we take the steady traveling wave ZND solution.

Fig. 1 shows the front evolution characteristic of the non-linear dynamics at the highest activation energy investigated of $E_a = 50$. The detonation first decouples to a quasi-steady shock followed by a decoupled reaction zone [14]. After the initial-re-initiation transient, the detonation re-ignites and proceeds with very irregular dynamics. It is these dynamics that we characterized.

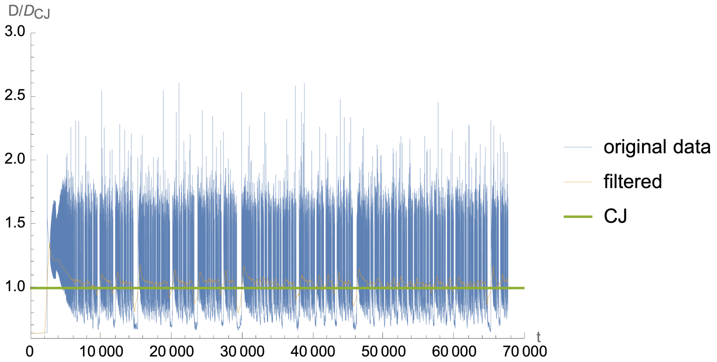

Figure 1: Shock speed evolution for the reactive Euler model with $E_a = 50$.

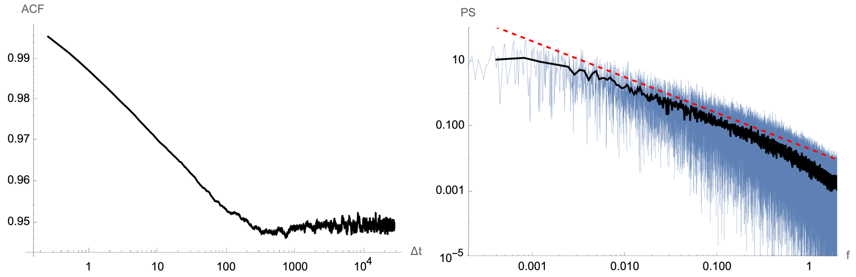

Figure 2: Auto-correlation (left) and power spectrum (right) of the signal of Fig. 1 in interval $[10000, 65000]$; red line denotes $1/f^{1.1}$ scaling, blue data is the power spectrum of the signal sampled at $\Delta t = 0.25$, black line uses 10000 non - overlapping partitions to cover the data-set.

The detonation lead shock speed evolution was first analyzed as a time-series using the auto-correlation function and the power spectrum. We usually omitted the initial transient, in this case for $t < 10000$. The auto-correlation function and power spectrum of the signal displayed in Fig. 1 are shown in Fig. 2. The auto-correlation is relatively flat. The flatness should not be confused with *white noise*, which would have a value of zero everywhere except at the origin. Indeed, the flatness is indicative of quite the opposite, a signal correlation on all scales, characteristic of SOC [15]. The signature of SOC is usually identified from the power spectrum by a $1/f$ scaling (which corresponds to a flat auto-correlation [15]). The power spectrum we record recovers the SOC scaling, with a best fit form of $1/f^{1.1}$. This illustrates quite convincingly that the dynamics follow a scale free organization to very large scales characteristic of SOC.

We have performed a preliminary investigation on the role of activation energy on the $1/f$ scaling of the power spectrum. For activation energies greater than 30, the power spectrum is found to scale as approximately $1/f$. The range of scaling grows with increasing activation energies. The final results will be provided at the conference.

We have also checked possible numerical issues, such as domain size and grid resolution. Our grid resolution recovered the bifurcation points of Henrick et al. [9]. Lower resolution results indicate these to have minor importance on the scaling of the power spectrum and only effected its very high frequency portion for $f \ll 1$ and restricted to the very high frequency instabilities associated mainly with the highly overdriven portions of the detonation front, where characteristic reaction times are shorter than the grid times. Detailed convergence studies will be provided at the conference. Domain size tests confirmed the very weak dependence on the rear boundary condition; see below.

In order to better understand the reason for SOC, we analyzed the dynamics of the detonations in terms of their spatio-temporal evolution. An example is shown in Fig. 3. The segment analyzed follows a punc-

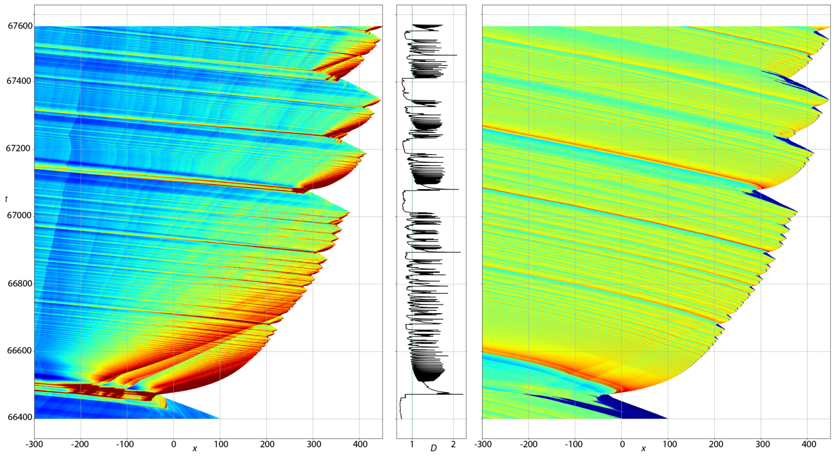

Figure 3: Space-time diagram of pressure (left) and temperature (right) evolution and front speed history (middle) for a data segment of Fig. 1.

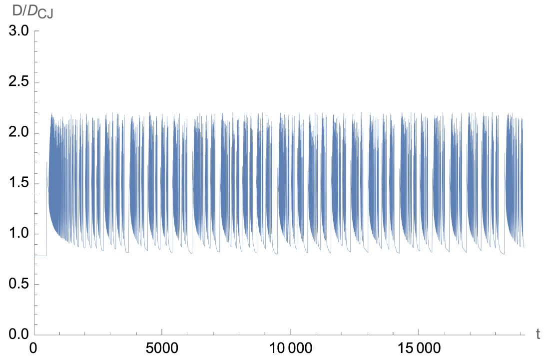

Figure 4: Shock speed evolution for in the Fickett detonation model with $E_a = 20$.

tuated failed event, followed by a sudden re-initiation. This re-initiation results in a highly overdriven detonation wave, which then decays as it is slowly eroded by the arrival of a long lived expansion wave originating from the end of the old fire. This is the classical dynamics of detonation pulsation [6,16,17], albeit here evolving on very long time scales owing to the large region separating the shock and decoupled fire. During this shock decay, owing to instability, new modes grow orders of magnitude faster than the long time decay of the main one, and the same process is repeated in a fractal-like structure at smaller and smaller scales.

3 SOC in Fickett detonations

We have also investigated the power spectra of irregular detonations predicted by the Fickett detonation model. The model is a reactive form of the non-linear one-way wave equation [6, 13, 18]. An example of shock dynamic evolution over very long times is shown in Fig. 4. The corresponding auto-correlation function and power spectrum are shown in Fig. 5. Nearly flat auto-correlation signals corresponding to a $1/f$ power spectrum were also observed for this system, strongly indicating SOC. The power spectrum we find scales as $1/f^{1.3}$. The slightly larger exponent in the Fickett model case than the Euler case signifies a more efficient energy transfer to low frequency modes.

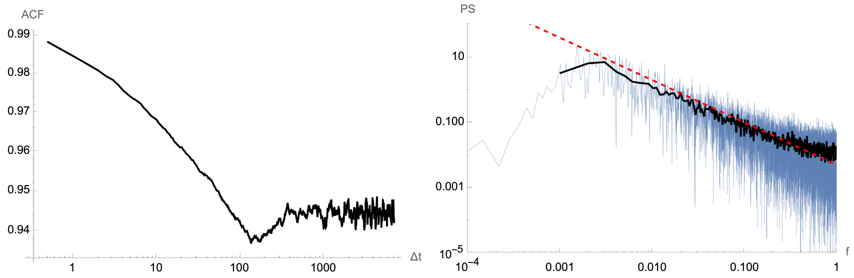

Figure 5: Auto-correlation (left) and power spectrum (right) of the signal of Fig. 4 in interval $[5000, 19000]$; red line denotes $1/f^{1.3}$ scaling, blue data is the power spectrum of the signal sampled at $\Delta t = 0.5$, black line uses 2000 non - overlapping partitions to cover the data-set.

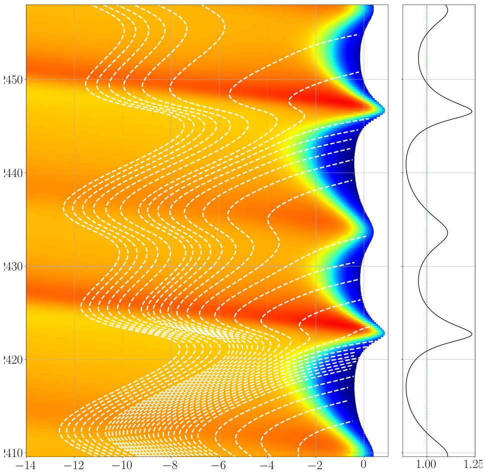

Figure 6: Space-time diagram of temperature evolution alomng with few characteristics paths for the period 2 instability of the reactive Euler equations for $E_a = 27.67$.

3 Further discussion

Our investigation of the spatio-temporal dynamics of pulsating detonations revealed the Russian-doll, fractal structure, whereby a hierarchy of instabilities are observed at different scales, each one embedded in the larger one. We find that this is compatible with the general picture we observe for detonations closer to the neutral stability boundary. Fig. 6 shows for example the dynamics of a mode 2 detonation, for $Ea = 27.67$. Forward facing characteristics are plotted to illustrate again the link between the dynamics of the front and the energy release behind the front. We find that the dynamics of the lower peaked mode are embedded into the dynamics of the longer period, higher amplitude oscillation.

The embedded dynamics of higher order modes into lower order ones suggests that the dynamics can be reconstructed conceptually by an asymptotic sequence of approximations, each closed individually, as suggested by Short [17]. We are currently pursuing this approach, investigating the predictions of our non-linear oscillator model developed for Fickett detonations [19]. We find the model predicts dynamics qualitatively in agreement with the SOC picture: a hierarchy of higher frequency small amplitude pulsations are embedded into larger amplitude and long duration pulsations, characterized by corkscrew like phase diagrams [19]. Power spectra predicted by the model are currently under investigation and results will be presented at the conference.

We note however that models presented are strictly one-dimensional, while real detonations are three-dimensional, even in narrow tubes. At present, while it is well known that the cellular structure is very irregular in hydrocarbon detonations, particularly methane, there is very limited knowledge on the hierarchy of scales, and the link between high frequency and low frequency cut-off scales on the dynamics. Much remains to be learned on the spatio-temporal dynamics of real detonations. Investigations of cellular detonations are underway in our laboratory.

4 Concluding remarks

Our investigation of the non-linear dynamics of detonations revealed a Russian-doll fractal like structure obeying SOC. While this opens up new avenues for modeling detonation waves, the established dynamics in detonations may also provide insight into other avalanche-like phenomena displaying SOC. It is important to note that our discovery of SOC is for a purely deterministic system. Traditionally, SOC is believed to be an emergent phenomenon connected with stochastic models with a very large number of degrees of freedom. Dynamics of detonations are thus sufficiently rich to display the same type dynamics as self-organized stochastic systems. Being deterministic, they offer a more physically transparent tool to study the emergence of SOC in their dynamics.

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