Nonlinear dynamics and chaos analysis of one-dimensional pulsating detonations

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Introduction

Since the pioneering work of Erpenbeck [1] and Fickett & Wood [2], the problem of one-dimensional detonation instability has been extensively studied both theoretically and numerically [3, 4, etc]. In recent years, a series of high-resolution numerical investigations of an idealized one-dimensional Chapman-Jouguet detonation has also been carried out by Sharpe [5-7] to carefully look at the long time evolution of the longitudinal instability and explore the nonlinear phenomena far from the stability limit. To this end, a general description of the large amount of results that is generated by such numerical simulations remains highly desirable.

In one-dimensional simulations, the detonation instability is manifested by the periodic longitudinal pulsation of the detonation front. Changes of a control parameter can cause the temporal pattern of the pulsation to pass from regularly periodic to higher irregular or chaotic structures. The oscillatory characteristics have indeed indicated a remarkable resemblance with a simple nonlinear oscillator [8]. This similarity also suggests that application of classical theories of nonlinear dynamics and chaos [9] may prove useful to interpret the time series data generated from the one-dimensional detonation simulations and provide insights into the physics of the detonation pulsating instability.

In the present study, long time numerical simulations of an idealized pulsating detonation with a simple one-step irreversible Arrhenius reaction kinetics are performed. The analysis attempts to draw the parallel between classical nonlinear systems and pulsating detonations from their similar dynamic characteristics. Results are interpreted using a variant of nonlinear dynamic concepts (e.g., bifurcation diagram, Lyapunov exponent, etc.) to characterize the phenomena behind the pulsating detonation.

Computational details and results

In order to simulate the long-time evolution of the pulsating detonation with high resolution, the one-dimensional reactive Euler equations are solved using a hierarchical adaptive second-order centered scheme [10]. An effective numerical resolution up to 128 points per half-reaction zone length of the steady ZND detonation is used to ensure the detailed features of the pulsating front are properly resolved. Results of the long-time evolution of the longitudinal instability (by passing all the initial transient) for varying activation energies E_a are given in figure 1, which show good agreement with previous results of Sharpe [5-7]. Hence, the present computation provides reliable raw data for further time-series analysis using different methods of nonlinear dynamics.

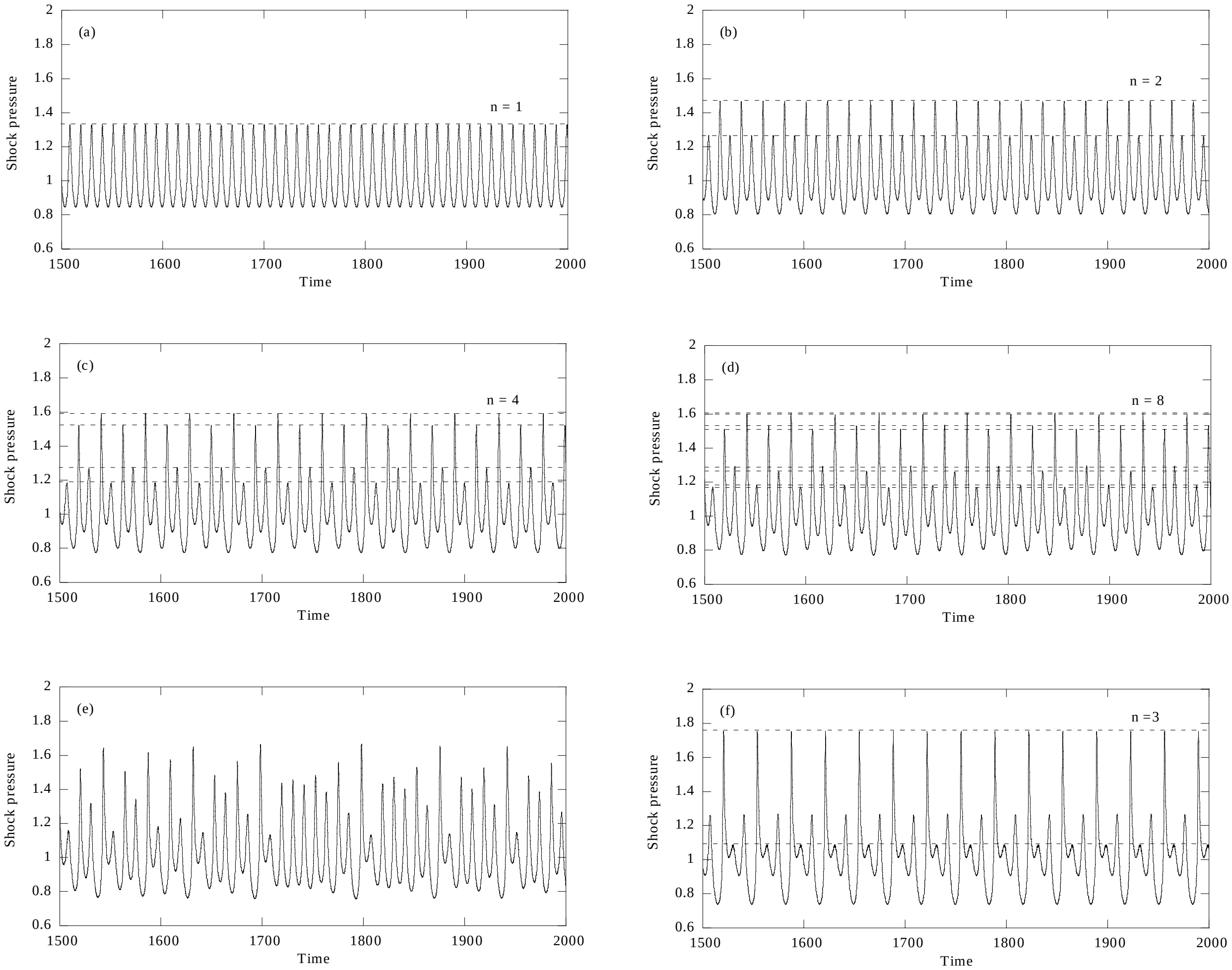

Figure 1. Shock pressure history for varying activation energies: (a) E_a = 27.00; (b) E_a = 27.40; (c) E_a = 27.80; (d) E_a = 27.82; (e) E_a = 28.00 and (f) E_a = 28.20.

Bifurcation analysis

Similar to previous numerical studies [4-7], the present results indicate that the cyclic pulsations change from harmonic oscillations to nonlinear and eventually to higher irregular oscillations as the value of the activation energy is systematically increased from its value at the stability limit. There have been several routes to chaos described in literature [9]. To illustrate the transition pattern, a bifurcation diagram has been constructed, as shown in figure 2. For each activation energy E_a, the local peaks in shock pressure of the pulsating detonation are measured by performing a global search of the time series, as signified by a change in slope and maximum among its eight neighbors. The principal features in this diagram are the vertical windows that correspond to ranges of the activation energy in which the solution is a stable periodic motion. The diagram indicates that the early stage of the pattern transition follows the period doubling route, i.e. the Feigenbaum sequence before the higher modes occur. The bifurcations come faster and faster until the system becomes aperiodic. Feigenbaum also discovered that the bifurcations should be occurring at a ratio that converged to a fundamental constant that is approximately 4.669 in a dynamical system. Some values of the Feigenbaum number for the present bifurcation diagram are shown in table 1, which also appear to approach to this universal value. The transition process of the pulsating front follows closely Feigenbaum's theorem for a simple nonlinear model with fewer degrees of freedom. From the bifurcation diagram, a narrow region of activation energy is found to contain a period 3 limit cycle, which suggests the solutions just to the left of this period 3 window should be chaotic [11].

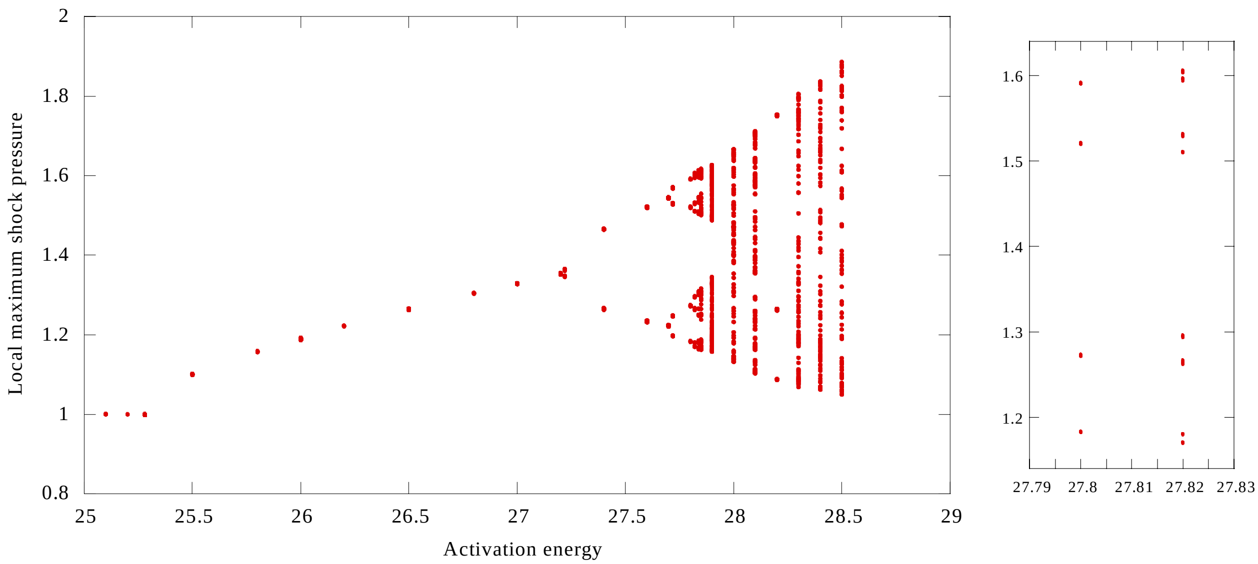

Figure 2. Bifurcation diagram of one-dimensional detonation for varying activation energies

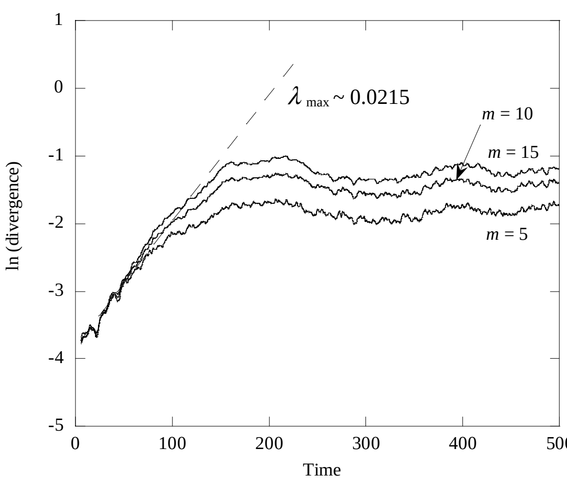

Figure 3. Plot of <ln (divergence)> versus time with different embedding dimensions m for the chaotic pulsation of detonation front with E_a = 28.00

Activation energy	Oscillation mode	Feigenbaum number
25.27	1	---
27.22	2	---
27.71	4	3.98
27.82	8	4.46
28.20	3	---

Table 1. Values of bifurcation limits and Feigenbaum numbers

Existence of chaos

There are several regions in the bifurcation diagram where highly aperiodic oscillations are found. These results can be further analyzed for the existence of deterministic chaos in the system. Detecting the presence of chaos in the system is important because of its relationship to other properties of the system concerned. One of the useful characterizations of chaos is provided by the Lyapunov exponent. It is a measure of the sensitivity of dependence on initial conditions. It quantifies the exponential rate of divergence of initially neighbouring phase-space trajectories and estimates the amount of chaos in a system. The divergence describes the rapid loss of the system's memory of its previous history as time evolves. For any time series in a dynamical system, the presence of a positive largest characteristic exponent leads to chaos. The algorithm used in the present study to calculate the largest Lyapunov exponent is due to Rosenstein *et al.* [12]. Figure 3 shows a typical plot of natural log of divergence versus time for the case of E_a = 28.00. The linear region means the divergence of nearest neighbors is exponential, where the slope can be interpreted as a measure of the largest Liapunov exponent. In this case, a positive Lyapunov exponent is found, which indicates the presence of chaos in the system and the system was sensitively dependent on initial conditions. In a more general sense, the Lyapunov exponent also provides another way to characterize whether the dynamical systems is likely to be unstable (if positive) or not (otherwise).

Concluding remarks

This paper presents preliminary analysis for the time series generated from numerical simulations of the one-dimensional detonations. The idea is to use standard techniques originally developed for nonlinear dynamics and chaos to understand different behaviors behind the pulsating detonation phenomena. Exploring these different nonlinear behaviors is important as it can serve to build models describing the complex detonation dynamics.

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