On the numerical computation of detonation instability

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1   Introduction

Instability is the hallmark of detonation. It is the reason for the fascinating oscillatory dynamics of one-dimensional gaseous detonations and for the beautiful cellular patterns in two or three-dimensional detonations [4, 11]. The detonation oscillations ranging from periodic to chaotic have been observed in numerical simulations of one-dimensional detonations since 1960s (see e.g. [5, 7, 12]). Cellular patterns are routinely observed both in experiments and numerical simulations [4, 11]. The principal questions that a theory of such phenomena must address are: 1) Can one reproduce the observations at a qualitative level and gain insight into the key physical mechanisms responsible for the observations? and 2) Can one predict the detonation dynamics at a quantitative level based on the first-principle modeling? Question 1) is obviously the easier of the two and research in this direction has enjoyed much success over the last half a century.

Concerning the theory of detonation instability, the rational analysis of the problem originates with the work of Erpenbeck [2, 3], which has subsequently been revisited by others [8–10, 14, 17, 21] (for more details, see the reviews [13, 15, 18] and references therein). Based on the extensive work done in the past, one might legitimately argue that the detonation stability theory has reached the state of maturity [15]. Indeed, it is *in principle* clear how to formulate the problem and what needs to be calculated [1, 2, 6, 15]. After all, the reactive Euler equations have been known for very long time. Linearization of the equations and of the shock conditions is a straightforward procedure. After the linearization, one needs to use, for example, the normal-mode substitution, and then solve the resulting eigenvalue problem numerically [10]. Alternatively, one can use the Laplace transform and again resort to numerics to invert the transform [3]. Already in 1962 [2], Erpenbeck wrote that "...to answer the question of stability in a specific case involves a rather large but apparently straightforward numerical computation". Surprisingly, however, not a single such calculation has ever been carried out for any case of a realistic gaseous detonation.

The reason is, of course, that *in practice*, the actual computations of detonation instability following this procedure are extremely difficult. The primary reason is numerical − the system of governing equations is in general very stiff and the computational procedure rather involved requiring repeated numerical solutions of stiff systems of ODE and a very large number of evaluations of various integrals. An additional source of difficulty is the far-field radiation condition that is necessary to ensure that the eigenvalue problem is well-posed (i.e. the eigenfunctions are bounded). The latter is a theoretical question that is still not completely settled, even though there is certainly some progress. As a result

of these difficulties, the only comprehensive computations that have been carried out so far are those for the perfect gas and the one-step Arrhenius kinetics (e.g. [10, 17]). Several results are available for simple models of multi-step kinetics and for more complex equations of state (e.g. [16]). But with the exception of [1] there are no published linear stability results for real mixtures wherein the detailed chemical mechanisms have been used. That is, from a practical point of view, the problem of predicting whether and how a given real mixture is unstable is, remarkably, still open. Erpenbeck's remark in [2] that "The conditions for stability of detonations, viz., that the zeros of $V(\tau)$ [1] have negative real parts, is of extraordinary complexity", remains valid today even though the normal-mode approach of Lee and Stewart [10] has considerably simplified the computations compared to that of Erpenbeck. Recently, methods based on the computation of Evans function have also been introduced [8] with some improvements on computational efficiency compared to the method of Lee and Stewart. But again, the success of the method has so far been limited to the idealized detonations.

Even though theoretical results on the instability of realistic detonations are lacking, direct numerical simulations of the reactive Euler equations that incorporate detailed chemical mechanisms indicate strongly that detonations are often unstable (see references in [11, 13]). However, such simulations are affected by severe numerical issues limiting their predictive power [20]. In particular, the problem of convergence is amplified in detonations due to the presence of strong instabilities, the wide range of spatial and temporal scales that must be resolved, and the possibility of chaotic dynamics [12]. The discrepancies between experiments and simulations raise many important questions as to the validity of the available chemical and thermodynamic data for the mixtures, the modeling framework of the reactive flows (Euler vs Navier-Stokes), and the numerical algorithms. In validating such simulation approaches, an important role is played by various theoretical results, such as exact solutions, which the simulations must be able to reproduce. In detonations with complex chemistry no such exact solutions are available, and the only feasible theoretical prediction that could be used is that of the linear stability. As such, these calculations can serve to benchmark the simulation codes. However, this is not the only value of the stability calculations. They provide valuable information about the nature of the instability in a given mixture that has implications for the nonlinear evolution of detonations. For example, if only few unstable eigenvalues exist, the detonation is expected to be rather regular, while the increased number of unstable eigenvalues is a sign of highly irregular detonations. Therefore, the linear stability calculations can serve to characterize explosive mixtures by their propensity to instability.

Thus, the fundamental question for the detonation stability theory, namely: How to efficiently and accurately predict the linear stability properties for a given mixture? is a question of a primarily algorithmic nature. Of course, this does not diminish its importance.

2   The linear stability problem

Within the framework of the reactive Euler equations, the detonation stability problem is in general posed as follows. Let the reactive Euler equations, say in two dimensions, be written as (e.g. [4])

$$\mathbf{v}_t + \mathbf{A}\mathbf{v}_x + \mathbf{B}\mathbf{v}_y = \mathbf{s}, \tag{1}$$

where $\mathbf{v} = \begin{bmatrix} \rho & \mathbf{u} & e & \mathbf{x} \end{bmatrix}^T$ is the solution vector, ρ is the fluid density, $\mathbf{u}$ is the fluid velocity, e is the energy, and $\mathbf{x}$ is the vector (say of size n) of the species concentrations. The matrices $\mathbf{A}$ and $\mathbf{B}$ and the source vector $\mathbf{s}$ are known functions of $\mathbf{v}$. These equations have a traveling-wave solution of the form $\mathbf{v} = \bar{\mathbf{v}}(x - Dt)$, where D is the wave speed that is to be determined. Substituting this ansatz into (1), we see that $\bar{\mathbf{v}}$ must solve the system of ODE,

$$(\mathbf{A}(\bar{\mathbf{v}}) - D\mathbf{I})\,\bar{\mathbf{v}}' = \mathbf{s}(\bar{\mathbf{v}}), \tag{2}$$

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[1]Erpenbeck's stability function

where $\mathbf{I}$ is the identity matrix. The steady detonation structure is such a solution of this system that contains a shock at say $x = 0$, gives $\bar{\mathbf{v}} = \mathbf{v}_a$ as the ambient-state constant solution ahead of the shock, $x > 0$, and a smooth profile solving (2) that satisfies the Rankine-Hugoniot jump conditions at $x = 0$, passes smoothly through a possible singularity of the matrix $\mathbf{A} - D\mathbf{I}$ at some point $x_* < 0$, and reaches the equilibrium state $\bar{\mathbf{v}} = \mathbf{v}_{eq}$ at $x \to -\infty$. Both the ambient and the equilibrium states must satisfy $\mathbf{s} = 0$ to be the solutions of (2). Usually, the ambient state is not an equilibrium (the cold boundary difficulty), hence $\mathbf{s}$ is forced to be zero at $x > 0$. The system (2) is solved then only in $x < 0$ subject to the conditions at equilibrium at $x \to -\infty$ and the shock conditions $\bar{\mathbf{v}}(0) = \mathbf{v}_s(\mathbf{v}_a, D)$, the latter known explicitly as functions of D and the ambient state.

When self-sustained (Chapman-Jouguet) detonations are considered, the matrix $\mathbf{A} - D\mathbf{I}$ is singular at the sonic point and certain regularity conditions must necessarily be satisfied there to ensure that the solutions of (2) remain smooth. These conditions will only be satisfied for particular values of D. Finding these values is itself a numerically involved process (due to the saddle-point character of the sonic point and the singular nature of the ODE (2)), but once D is found, the steady-state structure is completely determined. Subsequently, the problem of stability of such structure can be posed and solved, again numerically in general.

The linearization of the Euler equations is achieved by taking $\mathbf{v} = \bar{\mathbf{v}}(x) + \epsilon \mathbf{q}(x, y, t)$, substituting this expansion into (1), and collecting terms of $O(\epsilon)$. The result is a linear system [2]

$$\mathbf{q}_t + \bar{\mathbf{A}}\mathbf{q}_x + \bar{\mathbf{B}}\mathbf{q}_y = \bar{\mathbf{C}}\mathbf{q}, \tag{3}$$

which must be supplemented by the appropriate linearization of the shock conditions. Here $\bar{\mathbf{A}}$, $\bar{\mathbf{B}}$, and $\bar{\mathbf{C}}$ are matrices that depend on the steady-state solution and are hence functions of x.

Various existing algorithms differ by their approach to solving (3). Erpenbeck posed the initial value problem for $\mathbf{q}$ and solved it by the Laplace transform of $\mathbf{q}(x, y, t)$ in t and the Fourier transform in y. As a result, the transformed unknown $\hat{\mathbf{q}}(\tau)$ is a function of the Laplace-transform variable τ. He reduced the problem of the existence of instability to showing that a certain complex function $V(\tau)$ has roots with positive real part. This function $V(\tau)$ depends on the steady state solution as well as τ and it contains the entire information about the stability properties of a given mixture. Note that Erpenbeck's formulation [2] holds for rather general constitutive models. Nevertheless, the fact that fifty years later the approach has never been applied to any system more complex than the idealized one-step Arrhenius model, speaks of its prohibitively complex numerical nature.

Much more feasible computations are afforded by the normal-mode approach [10], which has been successfully extended to more complex systems than the one-step Arrhenius model. However, again, actual numerical implementation of the method for realistic mixtures remains as a theoretical possibility only with some partial results presently available [1].

3 A direct numerical approach

We propose to circumvent the difficulties mentioned above by completely abandoning the traditional approaches to the stability problem. The Laplace transform and the normal-mode methods are sensible and useful in handling simplified model problems. The small number of parameters that such models contain affords their systematic study and allows one to get important qualitative insight into the nature of the instability. For example, the computations in [10, 17] provided significant information on the role of the detonation overdrive, the activation energy, and the heat release on the structure of the unstable

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[2]We omit here certain technical details having to do with the choice of the frame reference and the appearance of the shock position in (3).
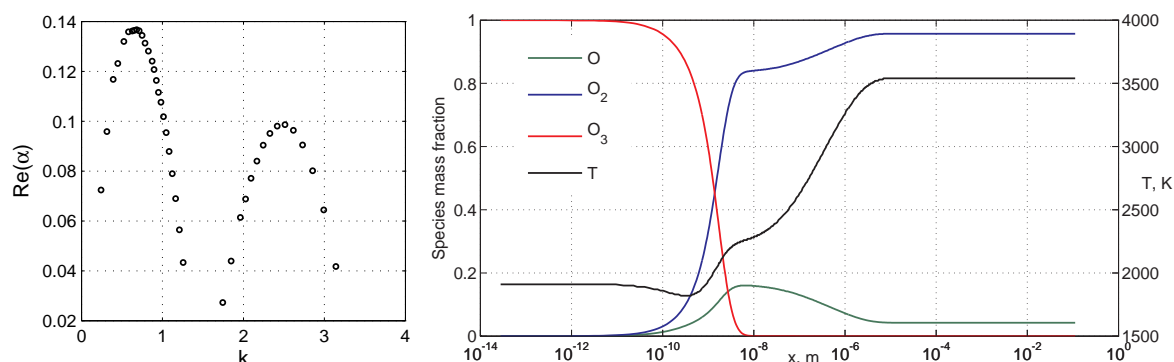
Figure 1: Left − computed spectra for the chain-branching model mechanism of [16]. Right − the steady structure of the ozone detonation displaying a wide range of spatial scales involved.

spectrum. However, technical difficulties associated with extending these methods to realistic systems remain prohibitive and motivate the search for alternative methods.

At present, numerical simulations of the reactive Euler equations can routinely be carried out with sophisticated and accurate algorithms (even though challenges remain when attempting to make quantitative predictions [20]). Somewhat paradoxically, it appears more difficult to solve the linear stability problem than to perform such nonlinear simulations. Because the numerical computation is a rather significant part of the linear stability theory in any case, one might argue for using the simulation algorithms to solve the stability problem directly, bypassing the normal-mode decomposition or the Laplace transform. Of course, as a result, significant amount of computations must be carried out, but despite such a drawback, the advantages of this approach are clear − it avoids altogether the algorithmic problems having to do with the computation of the Erpenbeck's function $V(\tau)$ or with the cumbersome computations required by the normal-mode algorithm.

Previously, such direct (however nonlinear) computations were carried out in [19] for two-dimensional idealized detonations. The shock-fitted algorithm presented in [19] is perfectly suited for the direct solution of the stability problem and is extended in the present work to handle realistic mixtures. In particular, here we consider the problem of detonation with a model three-step chain-branching chemistry [16] as a test case (Fig. (1)-left) and the problem of detonation in ozone with its full reaction mechanism consisting of three reversible reactions. Our previous calculations of the steady-state detonation structure in ozone reveal its severely multi-scale nature (Fig. (1)-right), which poses a challenge for numerical algorithms.

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