

# Accurate direct numerical computation of detonation instability

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## 1 Introduction

Numerical simulations of detonation have been conducted by many researchers over the years. Recently, methods of simulating detonations in a reference frame attached to the lead shock have been introduced [1, 2]. Rather than attempting to capture the evolving shock front numerically, as in conventional simulations, these shock-attached frame methods map the shock surface to a fixed location in the computational domain and solve for the shock state as part of the numerical solution. These methods allow a sharp representation of the lead shock by avoiding the numerical smearing or Gibbs oscillations inherent in shock capturing methods. Such shock fitting methods are ideal for the study of detonation instability since they are posed in the same frame of reference as considered in linear stability analysis, which allows for direct comparison of theoretical and numerical results. The main idea of the method was first proposed in [1], where the authors presented a one-dimensional shock mapping scheme that used the method of characteristics to advance the solution near the shock front and a shock capturing scheme in the region behind the shock. An alternative algorithm for advancing the shock state was proposed in [2]. Our present work follows these two previous publications and develops a method for general multi-dimensional detonation waves.

Soon after the experimental discovery that detonation waves are commonly unstable and tend to have a multi-dimensional structure, stability theories have been advanced, most notably by Erpenbeck, that have demonstrated that the reactive Euler equations predict instability of linear perturbations superimposed on the steady-state ZND solution (for a recent review of subsequent work on linear stability analysis, see [4]). The stability analysis is found to be rather abstruse and the research on the subject is still ongoing. While it has become commonplace in other areas of fluid dynamics to use high-resolution direct numerical simulation of the underlying governing equations to verify linear stability calculations (or vice versa), it has been a challenge to do the same in detonation science. The reasons can be found in both the difficulty of performing linear stability calculations and of obtaining sufficiently accurate simulation results. Although recent progress has allowed for sensitive calculation of the growth of detonation instability in one-dimensional simulations [1, 2], no results have appeared in the literature to validate the predictions of two-dimensional linear stability theory. This is primarily due to the tremendous resolution required to accurately measure these features using conventional shock-capturing

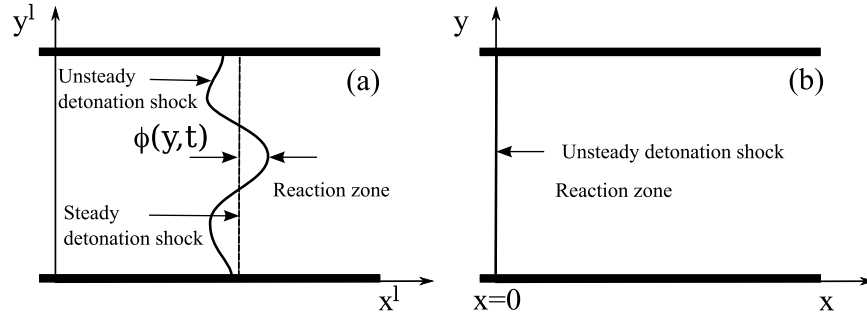


Figure 1: (a) Schematics of the perturbed detonation shock in the laboratory frame. (b) The computational domain after the perturbed shock has been mapped to  $x = 0$  in the shock-attached frame. The region to the right of the perturbed shock in (a) is mapped to the region  $x > 0$  in (b).

methods of simulation. In contrast, numerical simulations based on the shock-attached frame formulation described in the present work resolve these features very accurately even with moderate resolution.

## 2 Governing equations and numerical algorithm

We analyze detonation waves within the framework of the reactive Euler equations. The conservation form of the reactive Euler equations with a one-step chemical reaction is

$$\frac{\partial \mathbf{Y}}{\partial t^l} + \frac{\partial \mathbf{F}(\mathbf{Y})}{\partial x^l} + \frac{\partial \mathbf{G}(\mathbf{Y})}{\partial y^l} = \mathbf{S}(\mathbf{Y}), \quad (1)$$

where the superscript  $l$  denotes the laboratory frame, the vectors representing the state variables  $\mathbf{Y}$ ,  $x$ -fluxes  $\mathbf{F}$ ,  $y$ -fluxes  $\mathbf{G}$ , and the source term  $\mathbf{S}$  are

$$\mathbf{Y} = \begin{bmatrix} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho e_t \\ \rho \lambda \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} \rho u_1 \\ p + \rho u_1^2 \\ \rho u_1 u_2 \\ u_1 (\rho e_t + p) \\ \rho u_1 \lambda \end{bmatrix}, \quad \mathbf{G} = \begin{bmatrix} \rho u_2 \\ \rho u_1 u_2 \\ p + \rho u_2^2 \\ u_2 (\rho e_t + p) \\ \rho u_2 \lambda \end{bmatrix}, \quad \mathbf{S} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \rho \omega \end{bmatrix}. \quad (2)$$

In an ideal gas, the total energy density is  $e_t = pv/(\gamma - 1) - \lambda Q + \mathbf{u}^2/2$ , where  $\mathbf{u} = (u_1, u_2)$  is the particle velocity in the laboratory frame,  $p$  and  $v = 1/\rho$  are pressure and specific volume, respectively,  $\gamma$  is the ratio of specific heats,  $Q$  is the heat of reaction, and  $\lambda$  is the reaction-progress variable. A one-step, irreversible Arrhenius reaction rate law is used for the chemistry model:  $\omega = k(1 - \lambda) \exp(-E/pv)$ , where  $k$  is the pre-exponential rate constant, and  $E$  is the activation energy.

Our goal is to solve (1) for a detonation wave in a coordinate frame attached to the lead shock, so that we have only to calculate in the vicinity of the lead shock. Thus no calculation is done either in the unburnt gas ahead of the shock or in the region of burnt products too far behind the shock. Although it is possible to formulate the algorithm in general geometries, for the purpose of illustration, we consider a detonation propagating from right to left in a rectangular channel as shown in Figure 1. Let us make a coordinate transformation:  $x = x^l + D_0 t + \phi(y, t)$  and  $y = y^l$ , where  $D_0$  is the steady-state detonation velocity, and  $\phi(y, t)$  is the perturbation about the steady-state shock position. The abscissa,  $x$ , of the shock-attached frame is such that  $x = 0$  is the location of the shock at any time  $t$ . This is a coordinate transformation used in essentially all linear stability calculations of detonation [4]. Importantly, in stability theory,  $\phi$  is assumed small on the length scale of the reaction zone while in this work, we keep  $\phi$  general with the only proviso that it be a single-valued continuous function. Under

the above coordinate transformation, the governing equations become

$$\mathbf{Y}_t + \left[ \mathbf{F} + M v_a \sqrt{1 + \psi^2} \mathbf{Y} + \psi \mathbf{G} \right]_x + \mathbf{G}_y = \mathbf{S}, \quad (3)$$

preserving their conservation form. Two new variables, the normal mass flux across the shock,  $M(y, t)$ , and the shock slope,  $\psi = \phi_y$ , appear in the modified  $x$ -flux vector and hence an algorithm for their calculation is needed. Such an algorithm can be found by analyzing the Rankine-Hugoniot conditions and making use of the reactive Euler equations evaluated at the shock. One can show that the shock evolution (described by  $M$  and  $\psi$ ) obeys the system of equations,

$$\begin{bmatrix} M \\ \psi \end{bmatrix}_t + \begin{bmatrix} 0 \\ -v_a \sqrt{1 + \psi^2} M \end{bmatrix}_y = \begin{bmatrix} s \\ 0 \end{bmatrix}, \quad (4)$$

where  $s = s(M, \psi, \mathbf{q}) = (R_s - A_s)/A_0$ , and

$$A_0 = \frac{2}{\gamma + 1} M v_a \left( 3 + \frac{i_a}{M^2} \right), \quad R_s = (\gamma - 1) Q \rho_s \omega_s, \quad (5)$$

$$A_s = \rho_s [(c_s^2 - U_s^2) q_{11} + (c_s^2 - V_s^2) (q_{22} + \psi q_{21}) - U_s V_s (q_{12} + q_{21} + \psi q_{11})]. \quad (6)$$

Here  $q_{ij} = \partial u_i / \partial x_j$  are the components of the velocity-gradient tensor evaluated at the shock ( $(x_1, x_2) = (x, y)$ ) from inside the reaction zone,  $v_a = 1/\rho_a$  is the specific volume of the ambient unburnt state (subscript  $a$  denotes the ambient state,)  $i_a = \gamma p_a \rho_a$ ,  $p_a$  is the ambient pressure,  $c_s$  is the sound speed (subscript  $s$  denotes the shock state,) and  $U_s, V_s$  are the post-shock particle-velocity components in the shock-attached frame, which can be found as functions of  $M$  and  $\psi$  from Rankine-Hugoniot conditions. It is important to emphasize that (4) is exact and, provided that  $\mathbf{q}$  is known, is closed, that is: given  $\mathbf{q}$ , one can solve (4) for  $M$  and  $\psi$  from the initial and boundary conditions on  $M$  and  $\psi$ . Of course,  $\mathbf{q}$  is not known in general, but can be approximated from a previous time step in a numerical computation so that (4) can be solved over one time step.

At  $x > 0$ , i.e. within the reaction zone and in the following flow of products, we integrate (3) while at  $x = 0$  we integrate (4) and these two systems are coupled through  $\mathbf{q}$ . Spatial fluxes of the flow variables and the flux in the shock-slope equation were computed using a fifth-order WENO scheme. A third-order TVD Runge-Kutta scheme was used for temporal discretization. The velocity gradient tensor  $\mathbf{q}$  in the mass flux equation is computed using one-sided and centered finite-differences in the  $x$  and  $y$  directions, respectively, similar to that done in [2].

### 3 Results and discussion

One of our goals is to quantitatively verify the results of linear stability theory and to make use of the unique features of the shock-attached formulation to develop a method of analyzing the transverse detonation instability not only in the linear regime, but also in the subsequent non-linear regime. As with all calculations of stability, the results presented in this work are very sensitive. For example, the steady state solution is typically 5 to 10 orders of magnitude larger than the perturbations we seek to compute. Clearly, such small perturbations would be completely overwhelmed by shock-resolution errors of a shock-capturing method, but the present approach handles them nicely.

As an example, we consider initial data given by the steady one-dimensional ZND solution at  $\gamma = 1.2$ ,  $Q = 0.4$ ,  $f = 1$ , and  $E = 50$ . This detonation wave is one-dimensionally stable and two-dimensionally unstable over a small range of transverse disturbance wavenumbers [3]. Simulations were run at a typical resolution of 30 points per half-reaction zone length with the initially planar ZND solution perturbed by a sine wave of a given frequency. The growth rate and frequency of the instability were extracted by a least-squares fit of the solution to an exponential function. The dispersion relation thus constructed is shown in Figure 2(a). As one can see, there is an excellent agreement with linear stability theory.

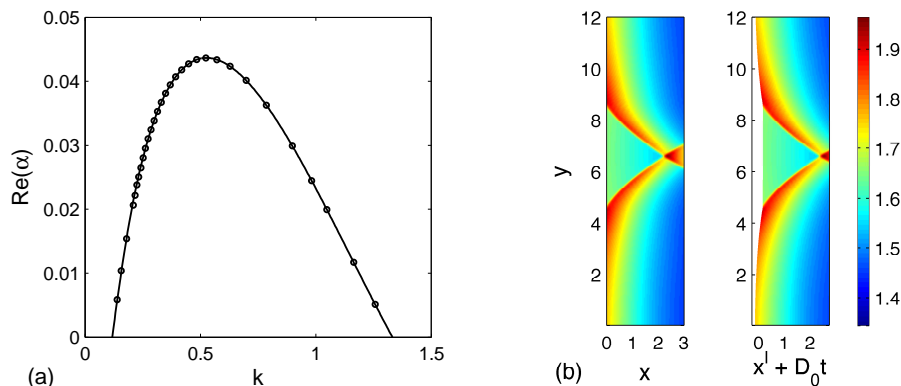


Figure 2: (a) Comparison of the theoretical dispersion relation (solid curve) with the one numerically computed by the present method (circles). (b) Comparison of the pressure field in the computational domain with the same in the physical space.

As the perturbations grow, they begin to deviate from exponential behavior predicted by the linear stability theory. Mode interactions and wave-breaking within the reaction zone lead to the formation of transverse shocks and eventually a full-fledged cellular detonation is formed. In Figure 2(b) we show the pressure field in the frame of the lead shock as computed by the numerical method (left) and the same field after mapping back to the physical domain (right).

One of the major advantages of the present method is that the numerical smearing errors or Gibbs oscillations near the lead shock are almost completely eliminated. Such errors only exist near the triple points after the cellular detonation has already appeared, while they are essentially absent in the linear regime and weakly nonlinear regime before the appearance of the transverse shocks.

Our ongoing work involves extending the method to strongly unstable detonations, as the present algorithm cannot handle strong triple-point configurations, and generalization to include complex chemical reactions and non-ideal equations of state.

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## References

- [1] A. R. Kasimov and D. S. Stewart. On the dynamics of self-sustained one-dimensional detonations: A numerical study in the shock-attached frame. *Phys. Fluids*, 16(10):3566–3578, 2004.
- [2] A. K. Henrick, T. D. Aslam, and J. M. Powers. Simulations of pulsating one-dimensional detonations with true fifth order accuracy. *J. Comput. Phys.*, 213(1):311–329, 2006.
- [3] M. Short and D. S. Stewart. Cellular detonation stability. part 1. a normal-mode linear analysis. *J. Fluid Mech.*, 525:161–192, 2005.
- [4] D. S. Stewart and A. R. Kasimov. State of detonation stability theory and its application to propulsion. *Journal of Propulsion and Power*, 22(6):1230–1244, 2006.