# Numerical Computation of Linear Stability of Detonations

Dmitry I. Kabanov

King Abdullah University of Science and Technology, Thuwal, Saudi Arabia Aslan R. Kasimov King Abdullah University of Science and Technology, Thuwal, Saudi Arabia and P.N. Lebedev Physical Institute of the Russian Academy of Sciences, Moscow, Russia

## **1** Governing equations

Linear stability of detonation waves is analyzed in this work by means of numerical calculation of timedependent solutions of linearized Euler equations. No assumption of normal modes is used which helps avoid solving singular systems of ordinary differential equations that arise in normal-mode analysis. Here we present the method for the case of one-dimensional flow of an ideal chemically reacting gas undergoing an irreversible reaction  $A \rightarrow B$ . The reaction progress is followed by a variable  $\lambda$  such that the mass fraction of A is  $1 - \lambda$  and that of B is  $\lambda$ .

In a reference frame attached to the lead shock which is assumed to propagate from left to right with timedependent speed D, the governing equations are written as

$$\rho_t + (\rho (u - D))_x = 0, (\rho u)_t + (\rho u (u - D) + p)_x = 0, (\rho e)_t + (\rho (u - D) e + pu)_x = 0, (\rho \lambda)_t + (\rho (u - D) \lambda)_x = \rho r.$$

where  $\rho$ , u, p, e, r are density, flow velocity, pressure, total specific energy, and reaction rate, respectively. The total specific energy is  $e = e_i + u^2/2$  with  $e_i = p/\rho (\gamma - 1) - Q\lambda$  denoting the internal specific energy for a calorically perfect gas with  $\gamma$  being the ratio of specific heats and Q the chemical heat release.

The numerical solution of the governing equations in the shock-attached frame requires an evolution equation for D. We use the equation derived in [7] specialized to one dimension:

$$\frac{dM}{dt} = s,\tag{1}$$

with

$$s = \frac{1}{A_0} \left( R_{\rm s} - A_{\rm s} \right), \qquad \qquad A_0 = \frac{2}{\gamma + 1} M v_{\rm a} \left( 3 + \frac{\gamma p_{\rm a} \rho_{\rm a}}{M^2} \right),$$
$$R_{\rm s} = Q(\gamma - 1) \rho_{\rm s} r_{\rm s}, \qquad \qquad A_{\rm s} = \rho_{\rm s} (c_{\rm s}^2 - U_{\rm s}^2) u_x |_{\rm s},$$

Correspondence to: aslankasimov@gmail.com

where  $M = -\rho_a D$  denotes the normal mass flux into the shock, v the specific volume, c the sound speed, U the fluid velocity in the shock-attached frame, and subscripts "a" and "s" denote ahead-of-shock and postshock quantities, respectively.

The following Rankine–Hugoniot conditions at x = 0 are used in the above expressions:

$$p_{\rm s} = -\frac{\gamma - 1}{\gamma + 1} p_{\rm a} + \frac{2v_{\rm a}}{\gamma + 1} M^2, \quad v_{\rm s} = \frac{\gamma - 1}{\gamma + 1} v_{\rm a} + \frac{2}{\gamma + 1} \frac{\gamma p_{\rm a}}{M^2}, \quad U_{\rm s} = M v_{\rm s}, \quad \lambda_{\rm s} = 0, \quad \rho_{\rm s} = \frac{1}{v_{\rm s}}.$$
 (2)

We introduce the vector of state variables  $z = (\rho, u, p, \lambda)^{\mathrm{T}}$  and linearize it as  $z(x, t) = \bar{z}(x) + z'(x, t)$  along with  $D(t) = \bar{D} + \psi'(t) = -\rho_{\mathrm{a}}(\bar{M} + M'(t))$ , with the bar denoting the steady-state values, and the prime the sought-for perturbation amplitudes. The resultant linearized governing equations in vector form are:

$$z'_{t} + A(\bar{z})z'_{x} + B(\bar{z})z' - \frac{d\bar{z}}{dx}\psi' = 0,$$
(3)

where

$$A(\bar{z}) = \begin{bmatrix} \bar{u} - \bar{D} & \bar{\rho} & 0 & 0\\ 0 & \bar{u} - \bar{D} & \frac{1}{\bar{\rho}} & 0\\ 0 & \gamma \bar{p} & \bar{u} - \bar{D} & 0\\ 0 & 0 & 0 & \bar{u} - \bar{D} \end{bmatrix}, \quad B(\bar{z}) = \begin{bmatrix} \frac{d\bar{u}}{dx} & \frac{d\bar{\rho}}{dx} & 0 & 0\\ -\frac{1}{\bar{\rho}^2} \frac{d\bar{p}}{dx} & \frac{d\bar{u}}{dx} & 0 & 0\\ C(\bar{\rho}\bar{r}_{\rho} + \bar{r}) & \frac{d\bar{p}}{dx} & \gamma \frac{d\bar{u}}{dx} + C\bar{\rho}\bar{r}_p & C\bar{\rho}\bar{r}_{\lambda}\\ -\bar{r}_{\rho} & \frac{d\bar{\lambda}}{dx} & -\bar{r}_p & -\bar{r}_{\lambda} \end{bmatrix},$$

and  $C = -Q(\gamma - 1)$  with subscripts  $\rho$ , p, and  $\lambda$  denoting partial derivatives.

Linearization of the Rankine–Hugoniot conditions (2) and the shock-evolution equation (1) yields:

$$p'_{s} = \frac{4v_{a}\bar{M}}{\gamma+1}M', \quad v'_{s} = -\frac{4\gamma p_{a}}{(\gamma+1)\bar{M}^{3}}M', \quad U'_{s} = \bar{M}v'_{s} + \bar{v}_{s}M', \quad \rho'_{s} = -\frac{v'_{s}}{\bar{v}_{s}^{2}}, \quad \lambda'_{s} = 0, \qquad (4)$$
$$\frac{dM'}{dt} = s', \qquad (5)$$

where

$$s' = \frac{1}{\bar{A}_0} (R'_{\rm s} - A'_{\rm s}) - \frac{A'_0}{\bar{A}_0^2} (\bar{R}_{\rm s} - \bar{A}_{\rm s}),$$
$$A'_0 = \frac{2}{\gamma + 1} \frac{3v_{\rm a}\bar{M}^2 - \gamma p_{\rm a}}{\bar{M}^2} M', \quad R'_{\rm s} = Q(\gamma - 1) \left[ (\bar{\rho}_{\rm s}\bar{r}_{\rho} + \bar{r}_{\rm s}) \,\rho'_{\rm s} + \bar{\rho}_{\rm s}\bar{r}_{p}p'_{\rm s} \right],$$
$$A'_{\rm s} = \rho_{\rm s} \left. \frac{d\bar{u}}{dx} \right|_{\rm s} \left[ \gamma \left( \bar{p}_{\rm s}v'_{\rm s} + \bar{v}_{\rm s}p'_{\rm s} \right) - 2\bar{U}_{\rm s}U'_{\rm s} \right] + \left( \bar{c}_{\rm s}^2 - \bar{U}_{\rm s}^2 \right) \left. \frac{d\bar{u}}{dx} \right|_{\rm s} \rho'_{\rm s} + \bar{\rho}_{\rm s} \left( \bar{c}_{\rm s}^2 - \bar{U}_{\rm s}^2 \right) u'_{x}|_{\rm s}.$$

The base steady-state solution is the ZND solution given by [7]:

$$\bar{v} = \frac{\gamma}{\gamma+1} \frac{P}{M^2} (1-\delta), \quad \bar{p} = P - M^2 \bar{v}, \quad \bar{U} = M \bar{v},$$

where

$$\delta = \sqrt{1 - \frac{hM^2}{P^2} \left(H + Q\bar{\lambda}\right)}, \quad h = \frac{2(\gamma^2 - 1)}{\gamma^2},$$

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and  $P = p_{\rm a} + \rho_{\rm a} D^2$ ,  $H = e_{\rm a} + p_{\rm a} / \rho_{\rm a} + D^2 / 2$ .

Now  $\overline{U}$ ,  $\overline{p}$ , and  $\overline{v}$  are defined in terms of  $\overline{\lambda}$  and D. To obtain the spatial structure, the rate equation for  $\overline{\lambda}$  is integrated starting at the shock with the initial condition  $\overline{\lambda}_s = 0$ .

For self-sustained detonations,  $D = D_{CJ}$ , where

$$D_{\rm CJ} = \sqrt{c_{\rm a}^2 + q} + \sqrt{q}, \quad q = \frac{(\gamma^2 - 1)Q}{2}, \quad c_{\rm a}^2 = \frac{\gamma p_{\rm a}}{\rho_{\rm a}}.$$

The preexponential factor k is defined such that the half-reaction length is unity:

$$k = \int_0^{1/2} \frac{\bar{U}}{\left(1 - \bar{\lambda}\right) \exp\left(-\frac{E_{\text{act}}}{\bar{p}\bar{v}}\right)} \, d\bar{\lambda}.$$

### 2 The numerical algorithm and results

To determine the stability properties of detonation for any particular set of parameters Q and  $E_{act}$ , we integrate (3) numerically. Each simulation result depends on the following numerical parameters: resolution per half-reaction zone  $N_{1/2}$ , closeness of  $\lambda$  to unity at the end of the reaction zone  $\tau_{\lambda}$ , and the amplitude of initial perturbation  $a_0$ . Once  $N_{1/2}$  and  $\tau_{\lambda}$  are specified, we compute the practical reaction zone length  $\mathcal{L}$ , for which  $0 \leq \lambda \leq 1 - \tau_{\lambda}$  rounded to the least succeeding integer, and discretize the domain using  $N = N_{1/2}\mathcal{L}$  grid points with coordinates  $x_i$ ,  $i = 0, \ldots, N$ , such that  $x_0 = -\mathcal{L}$  and  $x_N = 0$  are left and right boundary points, respectively. After this initialization step, simulation proceeds with the following steps: computation of ZND quantities, solution of the linearized system, and postprocessing.

Once the ZND quantities that enter the matrices A and B are found, we calculate the unsteady solution of the linearized system (3). The method of lines is used: on each time step we approximate spatial derivatives on the numerical grid thereby converting the system of PDEs to a system of ODEs and then evolving the latter in time:

$$\frac{dz'}{dt} = -\widehat{L}(\bar{z}, z', z'_x),\tag{6}$$

where  $\hat{L}(\bar{z}, z', z'_x)$  is an approximation of  $L(\bar{z}, z', z'_x) = A(\bar{z})z'_x + B(\bar{z})z' - \frac{d\bar{z}}{dx}\psi'$  from (3). We compute left- and right-biased approximations of the spatial derivatives  $z'_x$  based on the upwind method of the fifth order. Then  $\hat{L}$  is found using the global Lax–Friedrichs flux:

$$\widehat{L}(\bar{z}, z', z'_x) = L(\bar{z}, z', \frac{z'^-_x + z'^+_x}{2}) - \alpha \frac{z'^+_x - z'^-_x}{2},$$

where  $z'^{-}_{x}$  and  $z'^{+}_{x}$  are left- and right-biased approximations of  $z'_{x}$ , correspondingly,  $\alpha$  is the largest eigenvalue of A over the numerical grid:

$$\alpha = \max_{i=0,\dots,N+1} \{ \bar{u} - \bar{c}, \bar{u}, \bar{u} + \bar{c} \}|_{x=x_i}$$

Once  $\hat{L}$  is evaluated over the full grid, system (6) is evolved in time using the adaptive-step time integrator DOPRI5 [1], which is based on explicit Runge–Kutta method. We set both absolute and relative tolerances

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of the integrator to  $10^{-14}$ . Simulation proceeds to the final time  $T_{\rm f}$ , where typically  $T_{\rm f} = 10$  is used. While computing the solution, we record the time series of the perturbation of detonation velocity  $\psi'(t)$  at uniform time intervals  $\Delta t = 0.005$ . When simulation reaches  $T_{\rm f}$ , the solver computes the ratio of  $L_2$ -norms of the time series for  $T_{\rm f}/2 \le t \le T_{\rm f}$  and  $0 \le t \le T_{\rm f}/2$ , and if this ratio is smaller than three, then  $T_{\rm f}$  is increased to 100. The resulting time series of the detonation velocity allows us to extract growth rates and frequencies of perturbation by postprocessing.

At the beginning of each stage of the Runge–Kutta method, boundary conditions at the shock are specified using (4). Computation of approximations of  $z'_x$  near the boundaries of the computational domain is done as follows. Near the downstream boundary, we employ three ghost points and zero-order extrapolation, while near the upstream boundary (the shock) we use biased approximations of all the spatial derivatives, both in (3) and in (5), similar to that done in [2]. Initial condition for perturbation is specified by setting the perturbation of the detonation velocity  $\psi'$  to  $10^{-10}$  and flow variables z' to a multiple of the ZND solution such that  $\psi'$  and z' at the shock are consistent.

In the postprocessing step, the stability spectrum is extracted from the recorded time series  $\psi'(t)$ . The postprocessing algorithm is based on the Dynamic Mode Decomposition [4], which is a modern approach to extract low-dimensional dynamics based on exponentially growing and decaying oscillating modes from time series arising in numerical and experimental studies of fluid systems and in other fields as well.

To verify our approach, we compare the obtained instability spectra with the results known from the literature on normal-mode analysis of the same model [3, 5]. Table 1 shows the obtained results. These results demonstrate that the agreement of the spectra is at least to two significant digits. Besides growth rates and frequencies of modes, their relative errors are provided in this table computed by conducting simulations with two different grid resolutions and considering the results obtained with a finer resolution to be "true" results. Also, we were able to find a lower branch of the fundamental mode that was missing in [3], and later found in [5, 6]. For an example of the time series of the perturbation of detonation velocity, we consider detonation with  $\gamma = 1.2$ , Q = 50, and  $E_{act} = 26$ . This case was considered in [2] where one unstable mode  $\alpha = 0.03709980167992 + i 0.52214295442142$  was found by a least-squares fit of the time series of detonation velocity for early time of instability development in nonlinear simulations. Figure 1 shows an example of the time series of the perturbation of the detonation velocity that we obtain for this case from the unsteady linear computations with numerical parameters  $N_{1/2} = 40$ ,  $\tau_{\lambda} = 10^{-6}$ . Postprocessing of this time series gives one unstable mode  $\alpha = 0.03709 + i 0.52215$  with the relative error of the fit  $1.06 \times 10^{-5}$ . We see that four digits after decimal point are in agreement between the results obtained via the present approach and reported in [2]. Both Table 1 and the result described in this paragraph verify our approach and correctness of its implementation.

We also compute neutral stability curves for  $\gamma \in \{1.2, 1.3, 1.4\}$  using the present approach. Figure 2 displays the comparison between our computed results and those of [3, Figure 7] for the CJ case with  $\gamma = 1.2$ . A satisfactory agreement is seen. In Figure 3 we show the neutral boundary in Q-E plane (a) and the frequency of oscillation along the neutral boundary (b) for various  $\gamma$ . The smaller values of  $\gamma$  are seen to extend the range of unstable E to smaller E when  $Q \gtrsim 4$  and to reduce the unstable range towards larger values of E at  $Q \lesssim 4$ . At the same time, the frequency of neutral oscillation is seen to decrease substantially with decreasing  $\gamma$  at large Q while it is essentially independent of  $\gamma$  at small values of Q.

In computing the neutral stability curves, we generate 256 logspaced values of Q in the range  $10^{-0.35}$ – $10^2$ . For each Q we run simulations varying  $E_{act}$  according to an algorithm similar to the binary search algorithm until some particular value of  $E_{act}$  gives absolute value of the growth rate smaller than  $10^{-4}$ . For each Q

Table 1: Comparison of the stability spectra between the present work and the normal-mode results for  $\gamma = 1.2$  and Q = 50. Sources for the normal-mode results: \* [5, p. 2617]; \*\* [3, p. 127]. Description of columns: *i* is the mode number,  $\alpha_{re}$  growth rate,  $\alpha_{im}$  frequency,  $e_{re}$  relative error of growth rate,  $e_{im}$  relative error of frequency. Eigenvalues  $\alpha$  are in the scales used in the present work.

	_	Present work				Normal-mode analysis	
$E_{\rm act}$	i –	$\alpha_{\rm re}$	$e_{\rm re}$	$lpha_{ m im}$	$e_{\rm im}$	$\alpha_{\rm re}$	$lpha_{ m im}$
$25.26^{*}$	0 ·	-0.00017	$1 \times 10^{-4}$	0.53048	$6  imes 10^{-8}$	0.000	0.530
50.00**	$\begin{array}{c} 0.0\\ 0.1\\ 1\\ 2\\ 3\\ 4\\ 5\\ 6\\ 7\\ 8\\ 0\\ \end{array}$	$\begin{array}{c} 0.09365\\ 1.74458\\ 1.76536\\ 1.77399\\ 1.67745\\ 1.53541\\ 1.34788\\ 1.14096\\ 0.91468\\ 0.67788\\ 0.43002\\ \end{array}$	$\begin{array}{c} 3 \times 10^{-7} \\ 2 \times 10^{-11} \\ 6 \times 10^{-11} \\ 6 \times 10^{-12} \\ 1 \times 10^{-9} \\ 1 \times 10^{-8} \\ 4 \times 10^{-8} \\ 1 \times 10^{-7} \\ 5 \times 10^{-7} \\ 1 \times 10^{-6} \\ 4 \times 10^{-6} \end{array}$	$\begin{array}{c} 0.000\ 00\\ 0.000\ 00\\ 4.108\ 17\\ 7.830\ 05\\ 11.421\ 06\\ 14.993\ 13\\ 18.550\ 77\\ 22.105\ 24\\ 25.658\ 54\\ 29.211\ 39\\ 22\ 764\ 02\\ \end{array}$	$2 \times 10^{-16} \\ 2 \times 10^{-16} \\ 1 \times 10^{-12} \\ 2 \times 10^{-11} \\ 1 \times 10^{-10} \\ 4 \times 10^{-10} \\ 6 \times 10^{-10} \\ 7 \times 10^{-10} \\ 2 \times 10^{-10} \\ 2 \times 10^{-9} \\ 5 \times 10^{-9}$	N/A 1.743 1.764 1.772 1.676 1.534 1.346 1.140 0.913 0.677 0.421	N/A 0.000 4.104 7.823 11.42 14.98 18.53 22.09 25.64 29.19 22.72
	9 10	0.43092 0.17764	$\frac{4 \times 10}{2 \times 10^{-5}}$	32.70403 36.31692	$\frac{5 \times 10^{-8}}{1 \times 10^{-8}}$	0.431 0.177	32.73 36.28

the initial search range for critical  $E_{act}$  is [10; 140]. Other parameters are  $N_{1/2} = 40$  points and  $T_f = 10$ . Computation of each neutral stability curve took about 7 hours on 16-core machine. At the same time, for a typical single simulation not too far away from the neutral stability boundary and, say, numerical parameters  $N_{1/2} = 20$  and  $T_f = 100$ , time to solution is on the order of one minute.



Figure 1: Time series of the normalized detonation velocity for the detonation with parameters  $\gamma = 1.2$ , Q = 50, and  $E_{act} = 26$ .

Figure 2: The neutral stability curve computed with the present method and its comparison with the normal-mode result of Lee & Stewart [3, Figure 7].

Although we obtained some excellent results with the postprocessing algorithm based on DMD, we point out that making the algorithm robust is quite challenging in view of many control parameters that need



Figure 3: (a) The neutral stability curve at various  $\gamma$  and (b) frequency of oscillation  $\alpha_{im}$  along the neutral stability curves.

to be tuned to obtain the solution to desired accuracy. For example, the algorithm sometimes finds false eigenmodes, which, particularly, led to the situation where the algorithm of finding critical values of  $E_{act}$  did not converge at one point for the neutral stability curve for  $\gamma = 1.2$  shown on Figure 3.

In the ongoing work, we extend the present algorithm to more general situations that include the effects of multireaction kinetic mechanisms, presence of losses and two-dimensional effects. We intend to report on them in the near future.

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