Towards second-order algorithm for the pulsating detonation wave modeling in the shock-attached frame

Alexander I. Lopato, Pavel S. Utkin
Moscow Institute of Physics and Technology
Dolgoprudny, Moscow region, Russia
Institute for Computer Aided Design of the Russian Academy of Sciences
Moscow, Russia

1 Introduction

Numerous theoretical computational studies are devoted to the investigation of the mechanism of pulsating one-dimensional detonation wave (DW) propagation. As a rule, the researchers use the statement with a stationary DW propagating against the incoming flow and shock-capturing methods, for example see the list of references in [1]. Shock-capturing methods even of high approximation orders smear the leading shock wave (LSW) and the fact can lead to the qualitative changes in the DW propagation mechanism. For instance even for the theoretically stable DW shock-capturing methods provides high-frequency numerical oscillations of the peak pressure. The essentially different formulation includes the transition to the shock-attached frame [2, 3]. In this case the LSW becomes one of the boundaries of the fixed computational domain and so the problem of the LSW smearing is solved. However in the shock-attached frame one should introduce the shock speed evolution equation to define new unknown.

One of the main differences of the works [2] and [3] is the shock speed evolution equation formulation. In [3] the shock acceleration is connected with the momentum flux gradient at the shock and the approach seems to have troubles with strong internal shocks in strongly unstable detonations. In contrast the approach proposed in [2] demonstrates its applicability for the test with shock overtaking another shock. The goal of the work is re-formulation of the numerical algorithm from [2] in the finite volume manner, the increase of the approximation order of the shock speed evolution equation integration procedure from the first to the second, verification of the developed algorithm and numerical investigation of the main cases of the pulsating DW propagation using new algorithm.

2 Governing equations and numerical scheme

Following [2] write the reactive Euler equations in the shock-attached frame (x, t) where:

$$x = x^{lab} - \int_0^{t^{lab}} D dt,\ t = t^{lab}.$$

Correspondence to: pavel_utk@mail.ru

The superscript *lab* stands for the parameters in the laboratory frame. We consider the wave moving from left to the right, hence $x < 0$ is the region behind the leading SW. The governing equations in the vector conservative form are as follows:

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial}{\partial x}\left(\mathbf{f} - D\mathbf{u}\right) = \mathbf{s},$$

$$\mathbf{u} = \begin{bmatrix} \rho \\ \rho v \\ e \\ \rho Z \end{bmatrix}, \ \mathbf{f} = \begin{bmatrix} \rho v \\ \rho v^2 + p \\ (p+e)v \\ \rho v Z \end{bmatrix}, \ \mathbf{s} = \begin{bmatrix} 0 \\ 0 \\ -\rho Q \omega \\ \rho \omega \end{bmatrix}, \tag{1}$$

$$e = \rho\varepsilon + \frac{1}{2}\rho v^2, \ \varepsilon = \frac{p}{\rho(\gamma - 1)}, \ p = \frac{\rho}{\mu}RT, \ \omega = -A\rho Z \exp\left(-\frac{E}{RT}\right).$$

Here ρ is the total mixture density, v is the velocity in the laboratory frame, D is the shock speed, p is the pressure, e is the total energy density, Q is the heat release, ω is the reaction rate, Z is the mass fraction of a reactant, γ is the specific heat ratio, R is the universal gas constant, μ is the mixture molar weight, T is the temperature, A is the preexponential factor, E is the activation energy.

System of governing equations (1) was converted to the non-dimensional form in accordance to [4, 5]. Computational area is the interval $[-L; 0]$. Denote the total computational cells number as N. The right boundary corresponds to the LSW and the conditions are imposed as the Rankine-Hugoniot parameters corresponded to the current LSW speed (see the Section 3 below). On the left far boundary the zero-order extrapolation conditions are imposed. As it is known [6] the outflow boundary condition can significantly affect the results of pulsating DW modeling even for very long computational domains but we decided to concentrate on the investigation of various approximations for the right boundary conditions at the moment. The Zeldovich-von Neumann-Doring profiles are used as the initial conditions.

The computational algorithm is based on the physical processes splitting technique when on the time step at first the gas dynamics equations are integrated without taking into account chemical reactions ($\mathbf{s} = \mathbf{0}$) and then the chemical reactions are taken into account without convection terms [7]. The key point in gas dynamics equations integration procedure for the inner cells is the combination of (i) ENO-reconstruction approach [8] which is applied to build an interpolation polynomial for the local representation of grid function; (ii) monotone Courant-Isaacson-Rees numerical scheme in conservative formulation [9] rewritten in the shock-attached frame and (iii) Runge-Kutta time stepping [10]. Chemical kinetics equations for the reactant mass fraction and temperature are solved with the use of implicit Euler method.

3 The algorithm for the shock speed calculation

The shock-attached frame formulation of the governing equations leads to the modification of the numerical flux which includes now the unknown LSW speed D^{n+1} from the next time layer. The additional equations on the C_+-characteristics to calculate D^{n+1} are taken from [2]:

$$\frac{dx}{dt} = v + c - D, \ \frac{dp}{dt} + \rho c \frac{dv}{dt} - (\gamma - 1) Q \rho \omega = 0. \tag{2}$$

We use the local quadratic approximation for the characteristic curve $x(t) = at^2 + bt + c$ instead of linear one from [2] to increase the system (2) integration procedure approximation order (see Fig. 1). As the points $(0, t^{n+1})$, (x_*^n, t^n) and (x_*^{n-1}, t^{n-1}) belong to the parabola it is possible to express the parabola coefficients as the functions of x_*^n and x_*^{n-1}: $a = a(x_*^n, x_*^{n-1})$, $b = b(x_*^n, x_*^{n-1})$, $c = c(x_*^n, x_*^{n-1})$. The unknown x_*^n and x_*^{n-1} are found from the consideration of the first equation of (2). For the n-th and $(n-1)$-th time layers the equation is written as:

$$\begin{cases} 2a(x_*^n, x_*^{n-1})t^n + b(x_*^n, x_*^{n-1}) = v_*^n + c_*^n - D^n, \\ 2a(x_*^n, x_*^{n-1})t^{n-1} + b(x_*^n, x_*^{n-1}) = v_*^{n-1} + c_*^{n-1} - D^{n-1}. \end{cases} \quad (3)$$

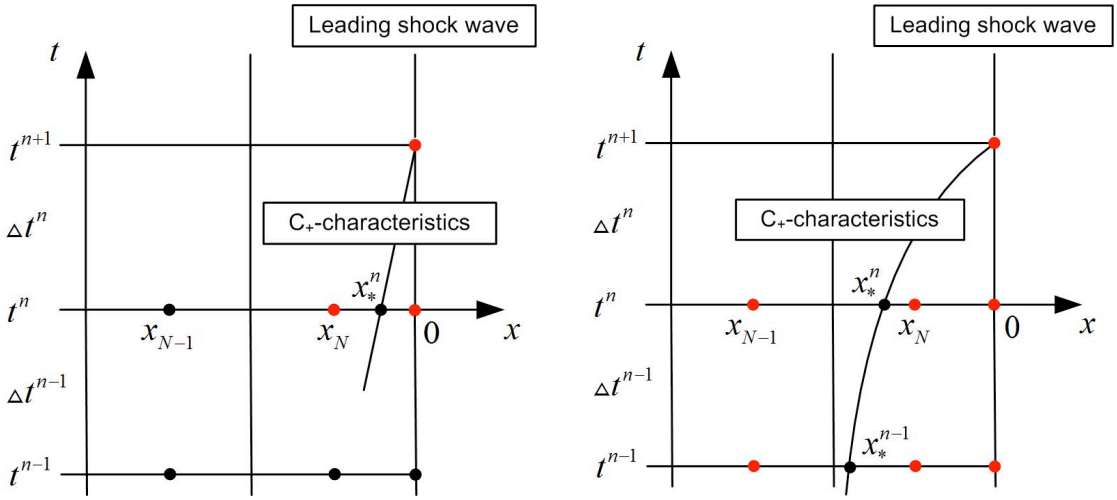


Figure 1. The sketch to the algorithm of the LSW speed equation integration – (a) finite volume formulation of the algorithm from [2], (b) developed algorithm of the second approximation order. Red dots denote the stencil in use.

Here gas velocity v_*^n and sound velocity c_*^n at the point (x_*^n, t^n) are expressed with the use of quadratic interpolation between points $(0, t^n)$, (x_N^n, t^n) and (x_{N-1}^n, t^n). Similarly the values $v_*^{n-1}(x_*^{n-1})$ and $c_*^{n-1}(x_*^{n-1})$ are expressed through the known values at the points $(0, t^{n-1})$, (x_N^{n-1}, t^{n-1}) and (x_{N-1}^{n-1}, t^{n-1}). System (3) is solved numerically with Newton iterations.

New LSW speed D^{n+1} is determined from the second equation of (2). We use three-point one-sided approximation of the derivatives *dp/dt* and *dv/dt* along the characteristics at the point $(0, t^{n+1})$:

$$\left(\alpha p_0^{n+1} + \beta p_*^n + \delta p_*^{n-1}\right) + \rho^{n+1} c^{n+1} \left(\alpha v_0^{n+1} + \beta v_*^n + \delta v_*^{n-1}\right) - (\gamma - 1) Q \rho^{n+1} \omega^{n+1} = 0,$$
$$\alpha = \frac{1}{\mathrm{V}t^n} + \frac{1}{\mathrm{V}t^n + \mathrm{V}t^{n-1}}, \ \beta = -\left(\frac{1}{\mathrm{V}t^n} + \frac{1}{\mathrm{V}t^{n-1}}\right), \ \delta = \frac{\mathrm{V}t^n / \mathrm{V}t^{n-1}}{\mathrm{V}t^n + \mathrm{V}t^{n-1}}. \quad (4)$$

Note that approximation (4) is suitable for the time integration with dynamic time stepping. The pressures at the points (x_*^n, t^n) and (x_*^{n-1}, t^{n-1}) again are calculated using quadratic interpolation procedure. All unknown values from the $(n+1)$-th time layer are expressed through the LSW Mach number M^{n+1} with the use of Rankine-Hugoniot conditions:

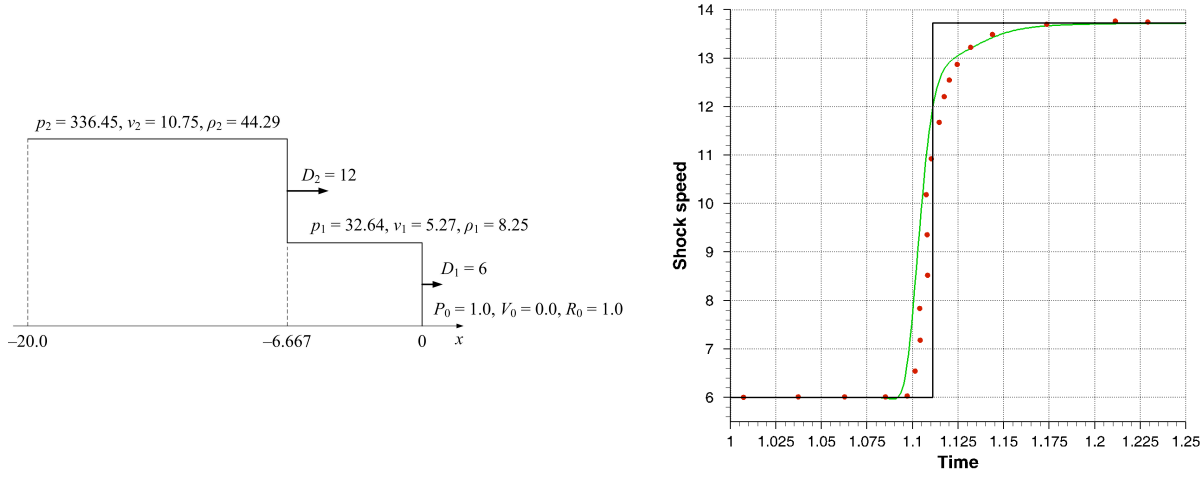
$$\frac{p_0^{n+1}}{P_0} = \frac{2\gamma}{\gamma+1}\left(M^{n+1}\right)^2 - \frac{\gamma-1}{\gamma+1}, \ \frac{\rho_0^{n+1}}{R_0} = \frac{(\gamma+1)\left(M^{n+1}\right)^2}{2 + (\gamma-1)\left(M^{n+1}\right)^2}, \ \frac{v_0^{n+1}}{C_0} = \frac{2}{\gamma+1}\frac{\left(M^{n+1}\right)^2 - 1}{M^{n+1}}, \ Z_0^{n+1} = 1, \quad (5)$$

where P_0, R_0 and C_0 are pressure, density and sound velocity before the DW. The gas is considered to be quiescent before the DW: $V_0 = 0$. Taking into account (5) the equation (4) is solved relative to M^{n+1} using Newton iterations. Obtained shock speed D^{n+1} is used then for the numerical flux calculation.

4 A shock overtaking another shock test

Consider the test case corresponded to that from [2] with a SW overtaking another SW in the inert gas. Fig. 2a illustrates the statement of the problem. The length of the computational area is L = 20.

Specific heat ratio is 1.25. The number of the computational cells is N = 500. Fig. 2b shows that the proposed approach is robust for the test in consideration, is almost free from the artificial pulsations and provides correct speed of the LSW after initial shock waves interaction. However the test is not good for the quantitative comparison of the developed algorithm with the original method from [2]. For this purpose the calculations of the main cases of the pulsating DW propagation – stable, weak unstable, irregular and strongly unstable cases – were carried out in the statements from [2] (see the Section 5 below).



(a) (b)

Figure 2. A shock overtaking another shock problem – (a) the exact statement from [2]; (b) shock speed dynamics at the time moment 0.15: black line – exact solution, green line – author's calculation, red dots – digitized solution from [2].

5 Pulsating detonation wave modeling

The numerical investigation of pulsating DW propagation was carried out for the fixed values of heat release Q = 50 and specific heat ratio γ = 1.2 and varied value of activation energy E. Chapman-Jouguet (CJ) speed for the chosen Q and γ is equal to $D_{CJ}^{theory} \approx 6.809475$. Fig. 3 demonstrates comparison of the obtained results with calculations from [2].

For the case of stable detonation we evaluated the real numerical algorithm approximation order as it was done in [3]. In calculation with cells number N = 4000 (see Fig. 3a) the LSW speed get the stable level $D_{CJ}^{calc1} \approx 6.809970$ at the time moment about 500, so the error in comparison with the exact CJ speed is:

$$\Delta_1 = \left| D_{CJ}^{theory} - D_{CJ}^{calc1} \right| \approx 0.000495.$$

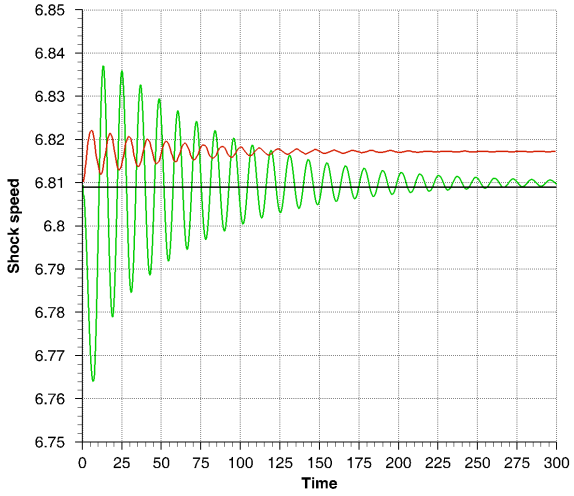
The calculation for the grid with cells number N = 2000 was also made. The stable LSW speed value for this case is $D_{CJ}^{calc2} \approx 6.811152$ and so:

$$\Delta_2 = \left| D_{CJ}^{theory} - D_{CJ}^{calc2} \right| \approx 0.001677.$$

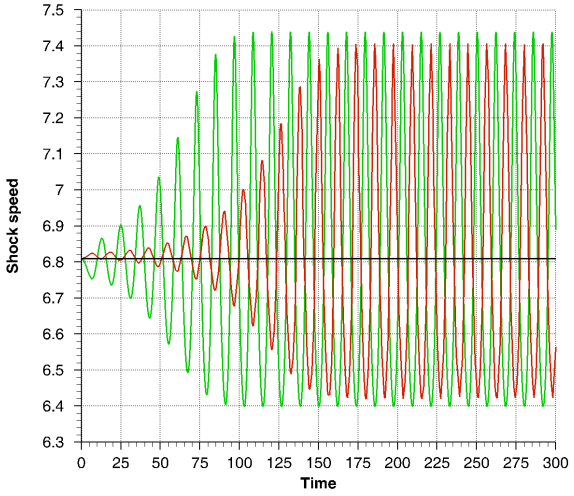
In accordance to the classical definition of the approximation order p:

$$p: \frac{\ln\left(\Delta_2 / \Delta_1\right)}{\ln 2} \approx 1.76.$$

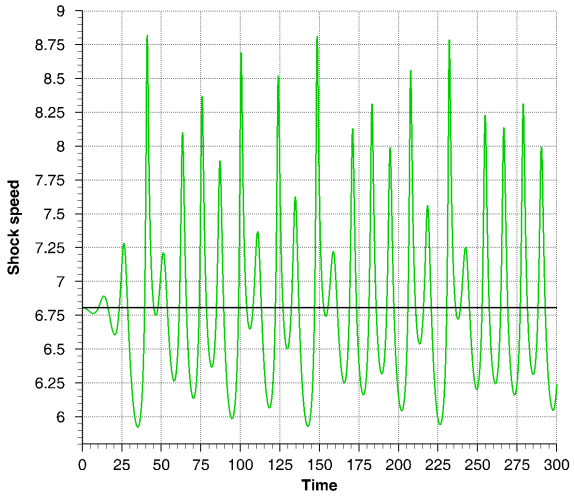
Such approximation order couldn't be reached using shock-captured methods and confirms the properties of the proposed algorithm.

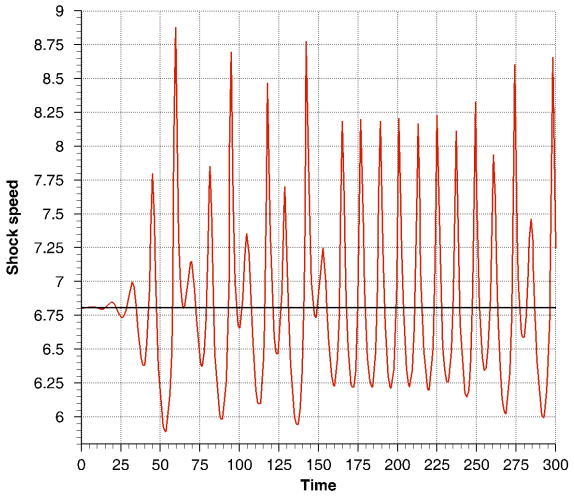


(a) $E = 25$, $N = 4000$, $L = 20$ – stable detonation

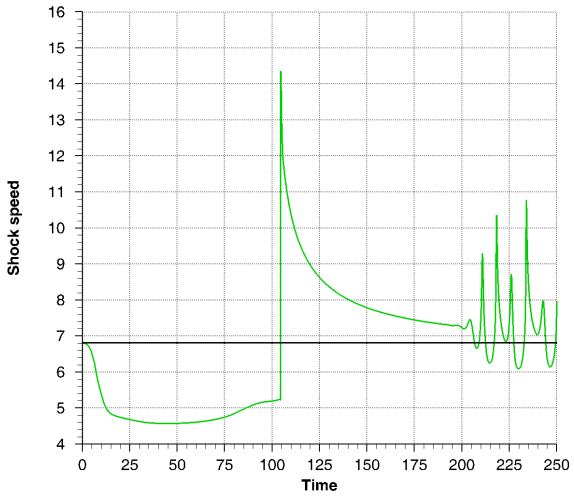


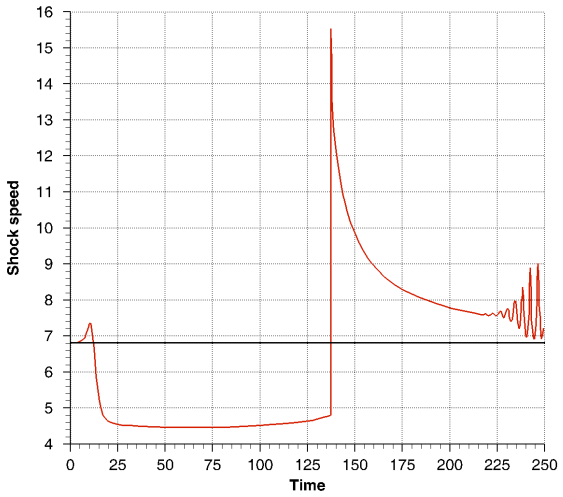
(b) $E = 26$, $N = 4000$, $L = 20$ – weakly unstable detonation





(c) $E = 28$, $N = 8000$, $L = 20$ – irregular detonation





(d) $E = 35$, $N = 16000$, $L = 60$ – strongly unstable detonation

Figure 3. LSW speed dynamics for the different cases of pulsating DW propagation. Green curves correspond to the author's calculations, red ones – digitized data from [2], black line – CJ speed level.

For the weakly unstable case the LSW speed reaches periodic limit cycle with the same frequency as in [2] but with slightly higher amplitude apparently due to the higher approximation order of the algorithm (see Fig. 3b).
The proposed algorithm is robust for the calculation of irregular (see Fig. 3c) and strongly unstable (see Fig. 3d) detonations.

Conclusions

We proposed the second approximation order numerical algorithm for the shock speed evolution equation integration which is necessary in case of pulsating detonation wave study in the shock-attached frame. The algorithm is based on the method of characteristics.
The algorithm and its realization are verified on the test with shock wave overtaking another shock. Results show the workability of the proposed approach.
The numerical investigations of pulsating detonation wave propagation in four cases – stable, weakly unstable, irregular and strongly unstable detonation – are carried out. For the stable case the estimated approximation order of the numerical algorithm is 1.76. The algorithm is robust for the cases of irregular and strongly unstable detonations.

Acknowledgements

Authors express their deep appreciation to Professor Aslan Kasimov for inspiration of the work and to KAUST University (Saudi Arabia) management for supporting meeting activity. This work is supported by the Russian Science Foundation under grant 14-50-00005 and performed in Steklov Mathematical Institute of Russian Academy of Sciences.

References

[1] Cole LK, Karagozian AR, Cambier J-L. (2012). Stability of flame-shock coupling in detonation waves: 1D dynamics. Comb. Sci. Tech. 184: 1502.

[2] Kasimov AR, Stewart DS. (2004). On the dynamics of the self-sustained one-dimensional detonations: A numerical study in the shock-attached frame. Phys. Fluids. 16: 3566.

[3] Henrick AK, Aslam TD, Powers JM. (2006). Simulations of pulsating one-dimensional detonations with true fifth order accuracy. J. Comp. Phys. 213: 311.

[4] Lee HI, Stewart DS. (1990). Calculation of linear detonation instability: one-dimensional instability of plane detonation. J. Fluid Mech. 216: 103.

[5] Semenko R, Faria L, Kasimov A, Ermolaev B. (2013). Set-valued solutions for non-ideal detonation. arXiv:1312.2180v1 [physics._u-dyn] 8 Dec 2013.

[6] Daimon Y, Matsuo A. (2003). Detailed features of one-dimensional detonations. Phys. Fluids. 15(1): 112.

[7] Toro EF. (2009). Riemann Solvers and Numerical Methods for Fluid Dynamics. Springer, 3rd ed. (ISBN 978-3-540-25202-3).

[8] Shu CW. (1997). Essentially non-oscillatory and weighted essentially non-oscillatory schemes for hyperbolic conservation laws. NASA/CR-97-206253, ICASE Report N 97-65.

[9] Kholodov AS. (1978). Construction of difference schemes with positive approximation for hyperbolic equations. USSR J. Comp. Math. and Math. Phys. 18(6): 116.

[10] Shu CW, Osher S. (1988). Efficient implementation of essentially non-oscillatory shock-capturing schemes. J. Comp. Phys. 77: 439.