MATHEMATICAL MODELING OF THE LONG-TIME EVOLUTION OF THE PULSATING DETONATION WAVE IN THE SHOCK-ATTACHED FRAME

Utkin P.S., Lopato A.I.
Institute for Computer Aided Design Russian Academy of Science
Moscow Institute of Physics and Technology

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What is detonation?

- **Detonation** is a hydrodynamic wave process of the supersonic propagation of an exothermic reaction through a substance.

- The **detonation wave (DW)** is a self-sustained shock wave (SW) discontinuity behind the front of which a chemical reaction is continuously initiated due to heating caused by adiabatic compression.

- The detonation wave velocities in gaseous mixtures under normal conditions are about **1 – 3 km/s**, front pressures – **10 – 50 atmospheres**.

Profile produced by gas motion behind the ideal detonation started at the closed end of the tube

Zeldovich – von Neumann – Doering (ZND) solution for the steady-state detonation

Detonation theory: state-of-the-art

**DW propagation is characterized by a complicated nonlinear oscillatory process**

- **1D.** *Pulsations* of parameters behind the DW front.
- **2D.** Transverse compression waves that interact with the DW in two-dimensional computations and experiments on the DWs propagation in narrow gaps. *Detonation cells.*
- **3D.** Transverse wave propagating in a spiral – *spin.*

![Graph](image1.png)


![Graph](image2.png)


![Graph](image3.png)

Detonation analogies and simplified models

Hydraulic jump and traffic jam are analogous to self-sustained DW (ZND-like front structures)


2D asymptotic equations:

\[\begin{align*}
    u_t + uu_x + v_y &= -\frac{1}{2} \lambda_x \\
    v_x &= u_y \\
    \lambda_x &= -k(1-\lambda)\exp\left[\theta\left(\sqrt{qu} + q\lambda\right)\right]
\end{align*}\]
Some problems in detonation calculations

Possibility of DW failure in the simulations of the DW long time propagation


Why does the detonation wave fail in the numerical computations?

Assumptions:

- Mistakes
- Mathematical models
- Computational method
The aim of the work – numerical investigation of weakly unstable and irregular regimes of pulsating DW propagation in two statements – the modeling of DW in the laboratory frame (LF) with detonation initiation near the closed end of the channel and modeling in the shock-attached frame (SAF), and quantitative comparison of results using Fourier analysis of the pulsations.
 Governing system of equations in the laboratory frame (LF)

\[
\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}}{\partial x} = \mathbf{s}
\]

\[
\mathbf{u} = \begin{bmatrix} \rho \\ \rho v \\ e \\ \rho Z \end{bmatrix}, \quad \mathbf{f} = \begin{bmatrix} \rho v \\ \rho v^2 + p \\ (p + e)v \\ \rho vZ \end{bmatrix}, \quad \mathbf{s} = \begin{bmatrix} 0 \\ 0 \\ -\rho Q\omega \\ \rho \omega \end{bmatrix}
\]

\[
e = \frac{1}{2} \rho v^2 + \rho \varepsilon, \quad \varepsilon = \frac{p}{\rho (\gamma - 1)}, \quad p = \rho \frac{R T}{\mu}, \quad \omega = -AZ \exp\left(-\frac{E}{RT}\right)
\]

1D Euler equations + one-stage chemical reaction model
Governing system of equations in the shock-attached frame (SAF)

\[ \tau = t \quad \xi = x - \int_0^t D dt \]

\[ \frac{\partial \mathbf{u}}{\partial \tau} + \frac{\partial}{\partial \xi} \left( \mathbf{f} - D \mathbf{u} \right) = \mathbf{s} \]

\[ \mathbf{u} = \begin{bmatrix} \rho \\ \rho v \\ e \\ \rho Z \end{bmatrix} \quad \mathbf{f} = \begin{bmatrix} \rho v \\ \rho v^2 + p \\ (p + e)v \\ \rho vZ \end{bmatrix} \quad \mathbf{s} = \begin{bmatrix} 0 \\ 0 \\ -\rho Q\omega \\ \rho \omega \end{bmatrix} \]

\[ e = \frac{1}{2} \rho v^2 + \rho \varepsilon \quad \varepsilon = \frac{p}{\rho (\gamma - 1)} \quad p = \rho \frac{RT}{\mu} \quad \omega = -AZ \exp \left( -\frac{E}{RT} \right) \]

1D Euler equations + one-stage chemical reaction model
+ shock velocity evolution equation
Brief review (shock-attached frame)

  - Numerical scheme: first approximation order scheme.
  - Shock speed evolution equation: integration of the governing equation along the $C_+$ characteristic near the shock.
  - Applicability: test with a shock overtaking another shock demonstrates the stability of the algorithm to detonation waves numerical calculations.
  - Results: main regimes of detonation wave propagation are obtained. The shock dynamics is shown to be determined entirely by the finite region between the shock and the sonic locus.

  - Numerical scheme: fifth approximation order WENO scheme + fifth order Runge-Kutta scheme.
  - Shock speed evolution equation: connecting with the momentum flux gradient.
  - Applicability: restrictions – strongly unstable detonation waves.
  - Results: the approximation order is shown to be equal to five (steady detonation). For an unstable regime a stable periodic limit cycle is obtained. The phase portrait confirms the unstable regime. The bifurcation diagram of different activation energies (different regimes) is constructed.
Dimensionless procedure

Characteristic scales – parameters in front of the DW and a half-reaction length:

\[ l_{1/2} = \frac{1}{1/2} \int_{1/2} u_{ZND}(Z) - D_{CI} AZ \exp \left(-E \rho_{ZND}(Z)/\rho_{ZND}(Z) \right) dZ \]

\[ \hat{\rho} = \frac{\rho}{\rho_a} \quad \hat{p} = \frac{p}{p_a} \quad \hat{u} = \frac{u}{u_a} \quad \hat{T} = \frac{T}{T_a} \quad \hat{\rho} = \frac{E}{\mu u_a^2} \quad \hat{Q} = \frac{Q}{u_a^2} \quad \hat{D} = \frac{D}{u_a} \quad \hat{l} = \frac{l}{l_{1/2}} \]

Dimensionless variables:

\[ \hat{A} = \frac{A}{u_a/l_{1/2}} = \frac{1}{1/2} \int_{1/2} \hat{u}_{ZND}(Z) - \hat{D}_{CI} AZ \exp \left(-E \hat{\rho}_{ZND}(Z)/\hat{\rho}_{ZND}(Z) \right) dZ \]

Dimensionless ZND profiles:

\[ \hat{u}_0(Z) = \frac{1}{\gamma + 1} \left( \frac{\hat{D}_{CI}^2 - \gamma}{\hat{D}_{CI}} \right) \left( 1 + \sqrt{Z} \right) \quad \hat{\rho}_0(Z) = \frac{\hat{D}_{CI}^2 + 1}{\gamma + 1} \left[ 1 + \frac{\hat{D}_{CI}^2 - \gamma}{\hat{D}_{CI}^2 + 1} \sqrt{Z} \right] \]

\[ \hat{\rho}_0(Z) = \left( \frac{\gamma}{\gamma + 1} \frac{\hat{D}_{CI}^2 + 1}{\hat{D}_{CI}^2} \left[ 1 - \frac{\hat{D}_{CI}^2 - \gamma}{\gamma (\hat{D}_{CI}^2 + 1) \sqrt{Z}} \right] \right)^{-1} \quad \hat{D}_{CI} = \sqrt{\frac{1}{2} \left( \sqrt{\hat{Q}}^2 - 1 \right) \hat{Q} + \frac{1}{2} \left( \sqrt{\hat{Q}} - 1 \right) \hat{Q}} \]


Computational algorithm

- Physical processes splitting technique
- Finite volume method
- Second approximation order ENO-reconstruction
- Courant-Isaacson-Rees numerical flux
- Second order Runge-Kutta explicit scheme for time stepping
- Euler implicit method for solving equations of energy and chemical reactions
- Parallelization (MPI)
- Algorithm of integration of the LSW velocity evolution (SAF)

\[
\begin{align*}
\mathbf{f}^{CIR}_{i+1/2} & = \frac{1}{2} \left[ \mathbf{f}\left( \{ \mathbf{u}^n_i \}^+ \right) + \mathbf{f}\left( \{ \mathbf{u}^n_{i+1} \}^- \right) \right] + \frac{1}{2} |A|^{n}_{i+1/2} \left[ \{ \mathbf{u}^n_i \}^+ - \{ \mathbf{u}^n_{i+1} \}^- \right] \\
|A|^{n}_{i+1/2} & = \frac{1}{2} \left[ \left( \Omega_i^n \right)^+ \left( \Omega_i^n \right)^{-1} \right] + \left( \Omega_{i+1}^n \right) \left( \Omega_{i+1}^n \right)^{-1}
\end{align*}
\]

Algorithm for shock speed calculation (1). SAF.

\[
\begin{align*}
\frac{d\xi}{d\tau} &= u + c - D \\
\frac{d\rho}{d\tau} + \rho \frac{du}{d\tau} - (\gamma - 1)Q\rho\omega &= 0
\end{align*}
\]

- Local quadratic approximation for the characteristic curve \( \xi(\tau) = a\tau^2 + b\tau + c \).
- Parabola coefficients are the functions of \( \xi^n, \xi^{n-1} \):
  \[
  a = a(\xi^n, \xi^{n-1}), \quad b = b(\xi^n, \xi^{n-1}), \quad c = c(\xi^n, \xi^{n-1}).
  \]
- From the first equation we find coordinates of two intersection points of characteristic curve with \( n \)-th and \( (n-1) \)-th time layers as the solution of the system:
  \[
  \begin{align*}
  2a(\xi^n, \xi^{n-1})\tau^n + b(\xi^n, \xi^{n-1}) &= u^n + c^n - D^n, \\
  2a(\xi^n, \xi^{n-1})\tau^{n-1} + b(\xi^n, \xi^{n-1}) &= u^{n-1} + c^{n-1} - D^{n-1}.
  \end{align*}
  \]
- The system is solved numerically with Newton iterations.
Algorithm for shock speed calculation (2). SAF.

\[
\frac{dp}{d\tau} + \rho c \frac{du}{d\tau} - (\gamma - 1) Q \rho \omega = 0
\]

- New LSW speed \( D^{n+1} \) is determined from the second equation.
- Three-point one-sided approximation of the derivatives:
  \[
  (\alpha p_0^{n+1} + \lambda p^o + \delta p_{n-1}^n) + \rho c^{n+1} (\alpha v_0^{n+1} + \lambda v_n + \delta v_{n-1}) - (\gamma - 1) Q \rho^{n+1} \omega^{n+1} = 0
  \]
  \[
  \alpha = \frac{1}{\Delta \tau^n} + \frac{1}{\Delta \tau^n + \Delta \tau^{n-1}}, \quad \lambda = \left(\frac{1}{\Delta \tau^n} + \frac{1}{\Delta \tau^{n-1}}\right), \delta = \frac{\Delta \tau^n / \Delta \tau^{n-1}}{\Delta \tau^n + \Delta \tau^{n-1}}.
  \]
- Calculation of the SW velocity \( D^{n+1} = M^{n+1} \cdot c^{n+1} \) on \((n+1)\)-th time layer as a solution of nonlinear equation. Here, Rankine-Hugoniot conditions are applied

\[
\frac{p_0^{n+1}}{p_0} = \frac{2\gamma}{\gamma + 1} \left(M^{n+1}\right)^2 - \frac{\gamma - 1}{\gamma + 1}, \quad \frac{p_0^{n-1}}{p_0} = \frac{(\gamma + 1) \left(M^{n+1}\right)^2}{2 + (\gamma - 1) \left(M^{n+1}\right)^2}, \quad \frac{v_0^{n+1}}{v_0} = \frac{2}{\gamma + 1} \left(M^{n+1}\right)^2 - 1, \quad z_0^{n+1} = 1.
\]

- Variables \( p^n, p_{n-1}^n, v^n, v_{n-1}^n \) are calculated using quadratic interpolation procedure.

Lopato A.I., Utkin P.S. Detailed simulation of the pulsating detonation wave in the shock-attached frame // Computational Mathematics and Mathematical Physics. 2016. 56.
Shock overtaking another shock test

\[ p_2 = 336.45, \quad v_2 = 10.75, \quad \rho_2 = 44.29 \]

\[ D_2 = 12 \]

\[ p_1 = 32.64, \quad v_1 = 5.27, \quad \rho_1 = 8.25 \]

\[ D_1 = 6 \]

\[ P_0 = 1.0, \quad V_0 = 0.0, \quad R_0 = 1.0 \]
Stable regime

\[ E = 25, \quad Q = 50, \quad \gamma = 1.2, \quad \Delta x = 5 \cdot 10^{-3} \]

\[ N_1 = 4000, \quad \Delta_1 = \left| \frac{p_{\text{calc1}}}{p_{\nu N}} - 1.0 \right| \approx 0.000150 \]

\[ N_1 = 2000, \quad \Delta_2 = \left| \frac{p_{\text{calc2}}}{p_{\nu N}} - 1.0 \right| \approx 0.000495 \]

\[ \left| \frac{p_{\text{calc}}}{p_{\nu N}} - 1.0 \right| \sim C \delta^k \quad k \approx \frac{\ln(\Delta_2/\Delta_1)}{\ln2} \approx 1.72 \]
Weakly unstable regime (1)

\[ E = 26, \ Q = 50, \ \gamma = 1.2, \ \Delta x = 5 \cdot 10^{-3} \]

\[ \Delta p \sim 10^{-4} \]

\[ T_{LF} = 11.79 \quad T_{LIN} = 12.11 \quad T_{SAF} = 11.85 \]

Weakly unstable regime (2)

\[ E = 26, \ Q = 50, \ \gamma = 1.2, \ \Delta x = 5 \cdot 10^{-3} \]

Long term numerical research
Weakly unstable regime (3)

\[ E = 26, \; Q = 50, \; \gamma = 1.2, \; \Delta x = 5 \times 10^{-3} \]

Fourier spectral analysis (5000 units of time)

\[
\frac{p}{p_{vn_0}} = \sum_{k=0}^{\infty} A_k \cdot \cos(2\pi v_k t)
\]
Weakly unstable regime (4)

- Fourier spectra of two statements demonstrate similar values of peak frequencies

<table>
<thead>
<tr>
<th>Peak</th>
<th>$v$ (LF)</th>
<th>$v$ (SAF)</th>
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<td>0</td>
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<td>9</td>
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<td>0.76133</td>
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Irregular regime (1)

\[ E = 28, \quad Q = 50, \quad \gamma = 1.2, \quad \Delta x = 2.5 \cdot 10^{-3} \]

\[ \Delta p \sim 10^{-4} \]

\[ \frac{p_{\text{peak}}}{p_{\text{vir}}} \]

\[ \frac{p_{\text{peak}}^{LF}}{p_{\text{vir}}} = \frac{1.65}{0.76} \]

\[ \frac{p_{\text{front}}}{p_{\text{vir}}} \]

\[ \frac{p_{\text{max}}^{SAF}}{p_{\text{min}}^{SAF}} = \frac{1.68}{0.76}. \]
Irregular regime (2)

\[ E = 28, \quad Q = 50, \quad \gamma = 1.2, \quad \Delta x = 2.5 \cdot 10^{-3} \]

Long term numerical research
Irregular regime (3)

\[ E = 28, \quad Q = 50, \quad \gamma = 1.2, \quad \Delta x = 2.5 \cdot 10^{-3} \]

Fourier spectral analysis (5000 units of time)

\[
\frac{p}{p_{vN}} = \sum_{k=0}^{\infty} A_k \cdot \cos(2\pi v_k t)
\]
Irregular regime (4)

- Fourier spectra of two statements demonstrate similar values of peak frequencies

<table>
<thead>
<tr>
<th>Peak</th>
<th>ω (LF)</th>
<th>ω (SAF)</th>
</tr>
</thead>
<tbody>
<tr>
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<td>0</td>
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<tr>
<td>4</td>
<td>0.33418</td>
<td>0.33464</td>
</tr>
</tbody>
</table>
Strongly-unstable regime (1)

\[ E = 35, \quad Q = 50, \quad \gamma = 1.2, \quad \Delta x = 3.75 \times 10^{-3} \]
Strongly-unstable regime (2)

\[ E = 35, \quad Q = 50, \quad \gamma = 1.2, \quad \Delta x = 3.75 \cdot 10^{-3} \]
1. The numerical investigation of pulsating DW propagation using two statements – laboratory frame and shock-attached frame – is carried out. The second statement includes the special numerical algorithm of the integration of shock speed evolution equation with the second approximation order based on the grid-characteristic method.

2. The calculation of the weak unstable mode gives a DW that tends to the stable limit cycle. Both statements give similar results that correlate with the known analytical solution. The spectral Furrier analysis demonstrates that main frequency peaks coincide although the regions between the peaks somewhat differ.

3. Numerical investigation of the irregular mode demonstrates the tendency of the front pressure reducing for laboratory statement. The spectral Furrier analysis confirms chaos presence.

4. Further investigations – long term calculation of strongly unstable mode for both statements.
1. Лопато, А.И., Уткин, П.С. Математическое моделирование пульсирующей волны детонации с
использованием ENO-схем различных порядков аппроксимации // Компьютерные
2. Лопато, А.И., Уткин, П.С. Особенности расчета детонационной волны с использованием схем
различных порядков аппроксимации // Математическое моделирование. – 2015. – Т. 27, № 7.
– С. 75 – 79.
3. Лопато, А.И., Уткин, П.С. О двух подходах к математическому моделированию детонационной

Lopato, A.I., Utkin, P.S. Two approaches to the mathematical modeling of detonation wave //

4. Лопато, А.И., Уткин, П.С. Детальное математическое моделирование пульсирующей
dетонационной волны в системе координат, связанной с лидирующим скачком // Журнал

Lopato, A.I., Utkin, P.S. Detailed simulation of the pulsating detonation wave in the shock-
attached frame // Computational Mathematics and Mathematical Physics. – 2016. – V. 56, No. 5.
– P. 841 – 853.

5. Лопато, А.И., Уткин, П.С. Towards second-order algorithm for the pulsating detonation wave
modeling in the shock-attached frame // Combustion Science and Technology. – 2016. – V. 188,
No. 11 (to appear).