International Conference Quasilinear equations, Inverse problems and their applications

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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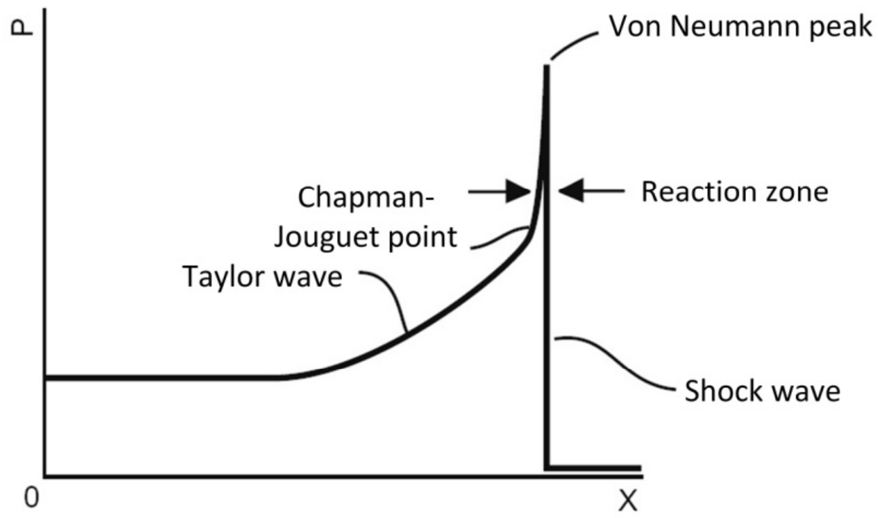
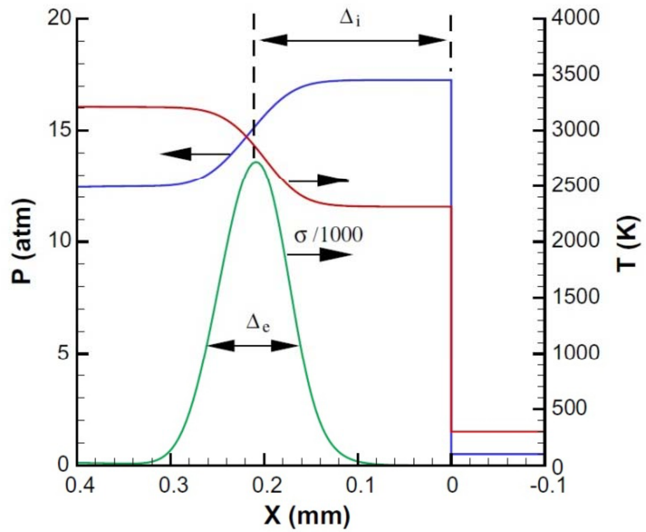
Moscow Institute of Physics and Technology, Dolgoprudny, 12 – 15 September 2016

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



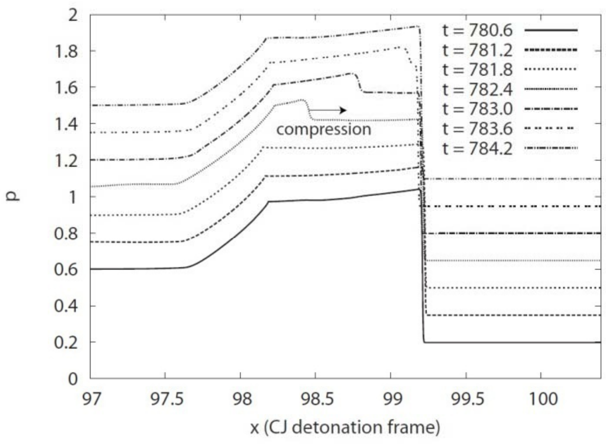
Zeldovich – von Neumann – Doering (ZND) solution for the steady-state detonation

Sheperd J.E. // Proc. Comb. Inst. 2009. 32.

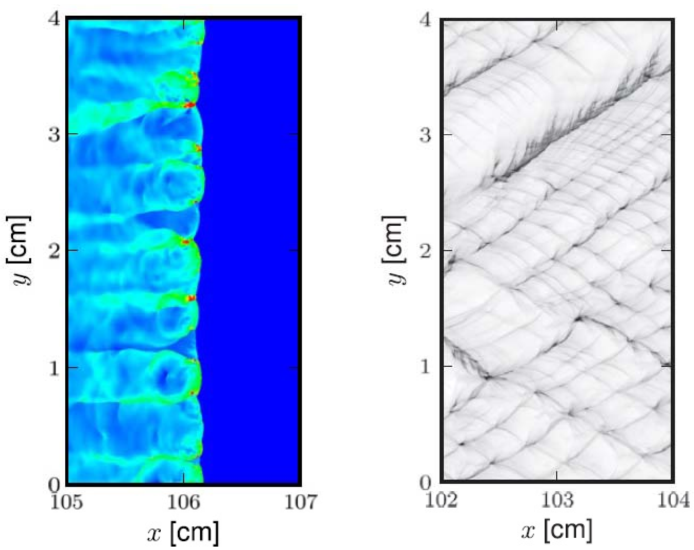
Detonation theory: state-of-the-art

DW propagation is characterized by a complicated nonlinear oscillatory process

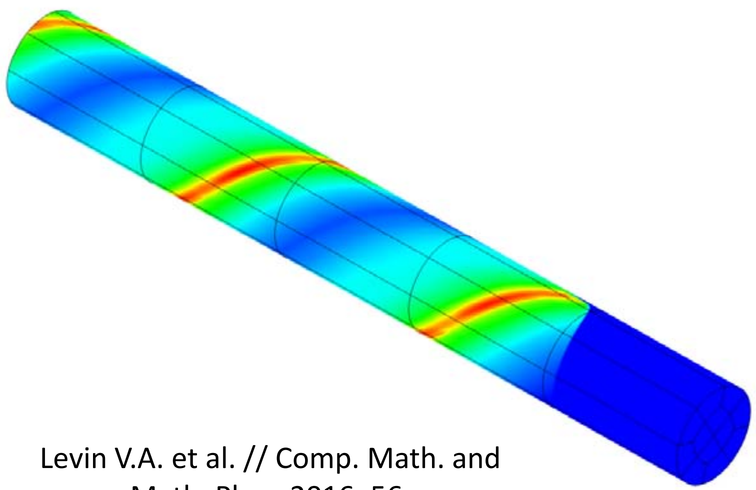
- **1D.** *Pulsations* of parameters behind the DW front.
- **2D.** Transverse compression waves that interact with the DW in two-dimensional computations and experiments on the DWs propagation in narrow gaps. *Detonation cells*.
- **3D.** Transverse wave propagating in a spiral – *spin*.



Leung C. et al. // Physics of Fluids. 2010. 22.



Taylor B.D. et al. // Proc. Comb. Inst. 2013. 34.

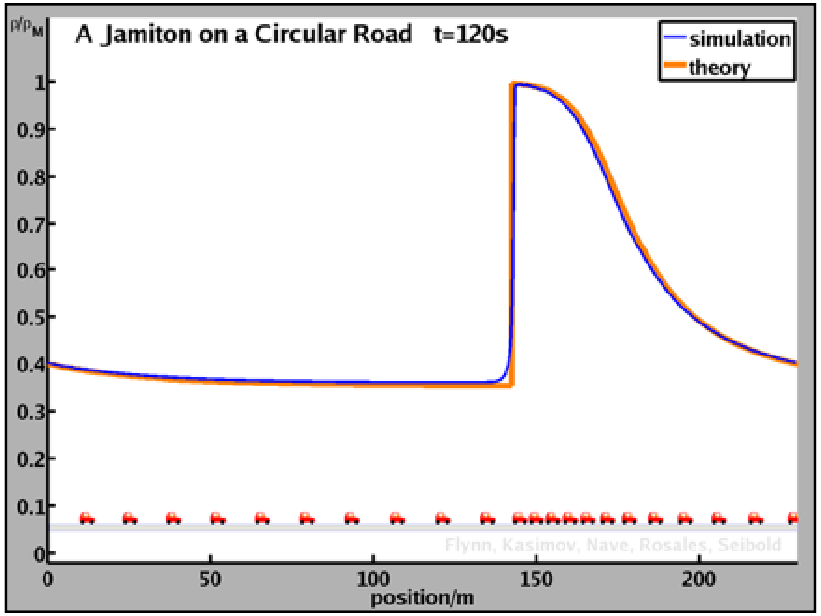


Levin V.A. et al. // Comp. Math. and Math. Phys. 2016. 56.

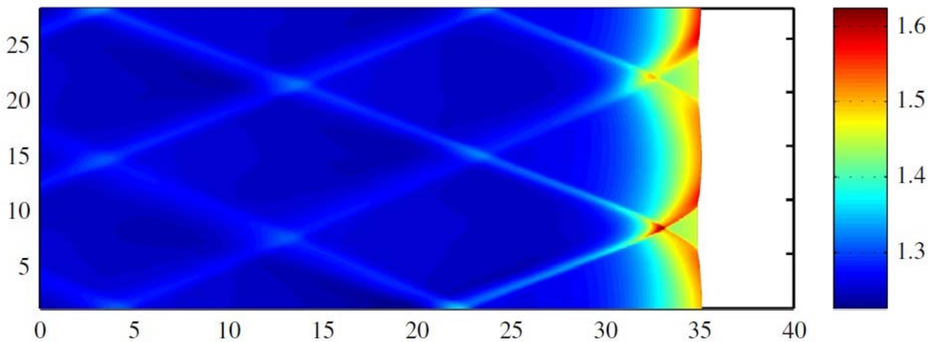
Detonation analogies and simplified models

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

Kasimov A.R. // J. Fluid Mech. 2008. 189.



Flynn M.R. et al. // Phys. Rev. E. 2009. 97.



2D asymptotic equations:

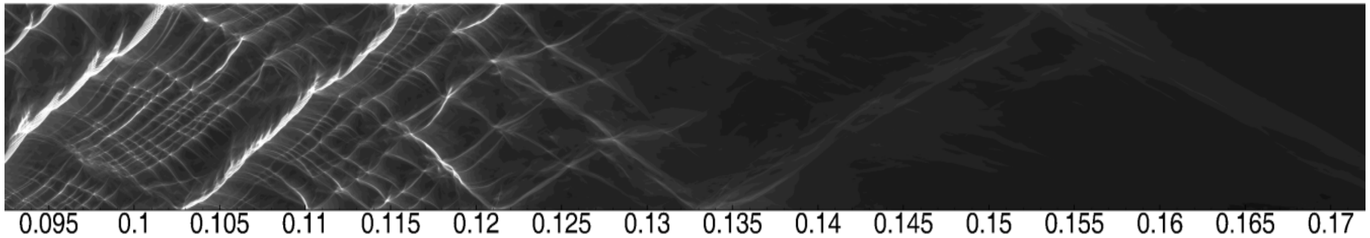
$$\begin{cases} u_t + uu_x + v_y = -\dfrac{1}{2}\lambda_x \\ v_x = u_y \\ \lambda_x = -k(1-\lambda)\exp\left[\vartheta\left(\sqrt{q}u + q\lambda\right)\right] \end{cases}$$

Faria L.M. et al. // J. Fluid. Mech. 2015. 784.

Some problems in detonation calculations

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

- Higgins A.J. Approaching detonation dynamics as an ensemble of interacting waves // Proc. 25th ICDERS. 2nd – 7th August 2015. Leeds, UK. Paper PL3.
- He L., Lee J.H.S. The dynamical limit of one-dimensional detonations // Physics of Fluids. 1995. 7.



Semenov I. et al. Mathematical modeling of detonation initiation via flow cumulation effects // *Progress in Propulsion Physics.* 8. Proc. EUCASS 2013. July 2013. Munich, Germany.

Why does the detonation wave fail in the numerical computations?

Assumptions:

- Mistakes
- Mathematical models
- Computational method

Aims

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**)

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

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

Z – mass fraction of the reacting mixture component
Q – heat release
A – pre-exponent factor
E – activation energy

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

1D Euler equations + one-stage chemical reaction model

Governing system of equations in the shock-attached frame (**SAF**)

$$\tau = t \qquad \xi = x - \int_0^t D\,dt$$

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

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

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1D Euler equations + one-stage chemical reaction model

+ shock velocity evolution equation

Brief review (shock-attached frame)

- Kasimov A.R., Stewart D.S. On the dynamics of the self-sustained one-dimensional detonations: A numerical study in the shock-attached frame // Physics of Fluids. 2004. 16(10): 3566 – 3578.
  - 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.

- Henrick A.K., Aslam T.D., Powers J.M. Simulations of pulsating one-dimensional detonations with true fifth order accuracy // Journal of Computational Physics. 2006. V. 213. P. 311 – 329.
  - 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 :

$$\rho_a \quad p_a \quad u_a = \sqrt{\frac{p_a}{\rho_a}} \quad T_a = \frac{p_a \mu}{\rho_a R}$$

$$l_{1/2} = \int_{1/2}^{1} \frac{u_{ZND}(Z) - D_{CJ}}{AZ \exp\left(-E\rho_{ZND}(Z)/p_{ZND}(Z)\right)} dZ$$

Dimensionless variables:

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

$$\hat{A} = \frac{A}{u_a / l_{1/2}} = \int_{1/2}^{1} \frac{\hat{u}_{ZND}(Z) - \hat{D}_{CJ}}{Z \exp\left(-\hat{E}\hat{\rho}_{ZND}(Z)/\hat{p}_{ZND}(Z)\right)} dZ$$

Dimensionless ZND profiles:

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

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

Erpenbeck J.J. Stability of steady-state equilibrium detonations // Physics of Fluids. 1962. V. 5. P. 604 – 614.

Semenko R. et al. Set-valued solutions for non-ideal detonation // Shock waves. 2016. V. 26. P. 141 – 160.

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)

$$\mathbf{f}_{i+1/2}^{CIR} = \frac{1}{2}\left[\mathbf{f}\left(\left\{\mathbf{u}_i^n\right\}^+\right) + \mathbf{f}\left(\left\{\mathbf{u}_{i+1}^n\right\}^-\right)\right] + \frac{1}{2}\left|A\right|_{i+1/2}^n \left[\left\{\mathbf{u}_i^n\right\}^+ - \left\{\mathbf{u}_{i+1}^n\right\}^-\right]$$

$$\left|A\right|_{i+1/2}^n = \frac{1}{2}\left[\left\{\Omega_i^n \left|\Lambda_i^n\right| \left(\Omega_i^n\right)^{-1}\right\}^+ + \left\{\Omega_{i+1}^n \left|\Lambda_{i+1}^n\right| \left(\Omega_{i+1}^n\right)^{-1}\right\}^-\right]$$

Lopato A.I., Utkin P.S. // Comp. Research Model. 2014. 6.

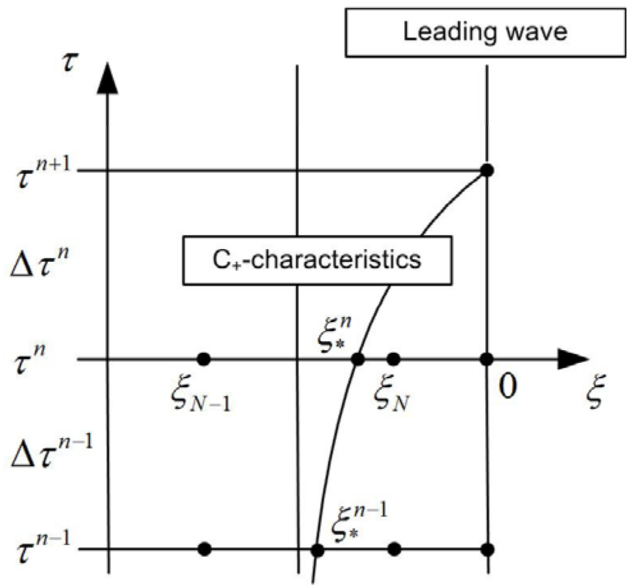
Algorithm for shock speed calculation (1). SAF.

$$\begin{cases} \dfrac{d\xi}{d\tau} = u + c - D \\ \dfrac{dp}{d\tau} + \rho c \dfrac{du}{d\tau} - (\gamma - 1) Q \rho \omega = 0 \end{cases}$$

- **Local quadratic approximation for the characteristic curve $\xi(\tau)$: $\xi(\tau) = a\tau^2 + b\tau + c$.**
- **Parabola coefficients are the functions of ξ_*^n, ξ_*^{n-1} :**
  $a = a\left(\xi_*^n, \xi_*^{n-1}\right),\ b = b\left(\xi_*^n, \xi_*^{n-1}\right),\ c = c\left(\xi_*^n, \xi_*^{n-1}\right).$
- **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:**

$$\begin{cases} 2a\left(\xi_*^n, \xi_*^{n-1}\right)\tau^n + b\left(\xi_*^n, \xi_*^{n-1}\right) = u_*^n + c_*^n - D^n, \\ 2a\left(\xi_*^n, \xi_*^{n-1}\right)\tau^{n-1} + b\left(\xi_*^n, \xi_*^{n-1}\right) = u_*^{n-1} + c_*^{n-1} - D^{n-1}. \end{cases}$$

- The system is solved numerically with Newton iterations.



Algorithm for shock speed calculation (2). SAF.

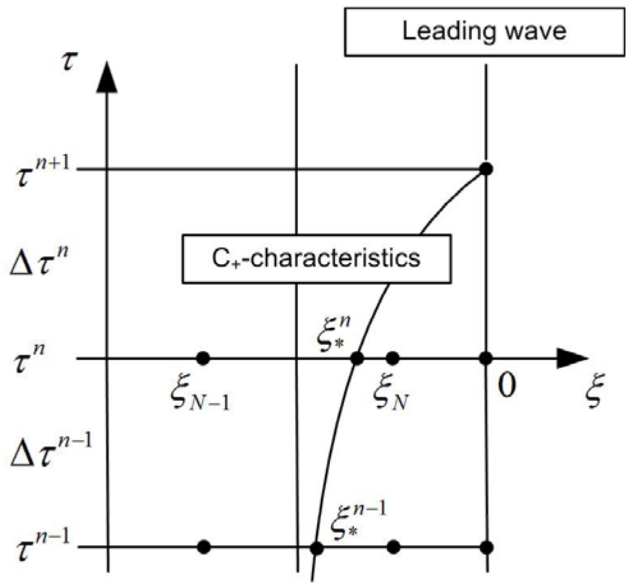
$$\frac{dp}{d\tau}+\rho c\frac{du}{d\tau}-(\gamma-1)Q\rho\omega=0$$

- New LSW speed D^{n+1} is determined from the second equation.

- Three-point one-sided approximation of the derivatives:

$$\left(\alpha p_0^{n+1}+\lambda p_*^n+\delta p_*^{n-1}\right)+\rho^{n+1}c^{n+1}\left(\alpha v_0^{n+1}+\lambda v_*^n+\delta v_*^{n-1}\right)-(\gamma-1)Q\rho^{n+1}\omega^{n+1}=0$$

$$\alpha=\frac{1}{\Delta\tau^n}+\frac{1}{\Delta\tau^n+\Delta\tau^{n-1}},\ \lambda=-\left(\frac{1}{\Delta\tau^n}+\frac{1}{\Delta\tau^{n-1}}\right),\ \delta=\frac{\Delta\tau^n/\Delta\tau^{n-1}}{\Delta\tau^n+\Delta\tau^{n-1}}.$$



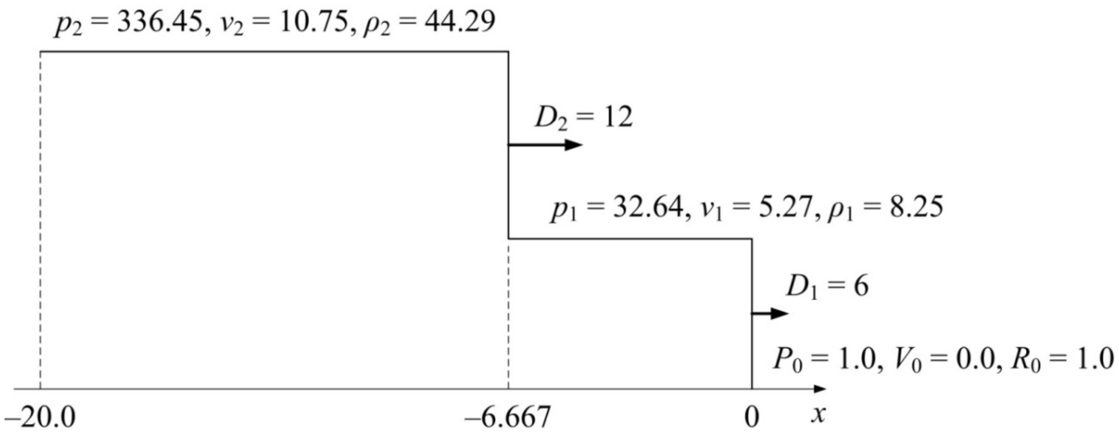
- Calculation of the SW velocity $D^{n+1} = M^{n+1} \cdot c^{n+1}$ on (n+1)-th time layer as a solution of nonlinear equation. Here, Rankine-Hugoniot conditions are applied

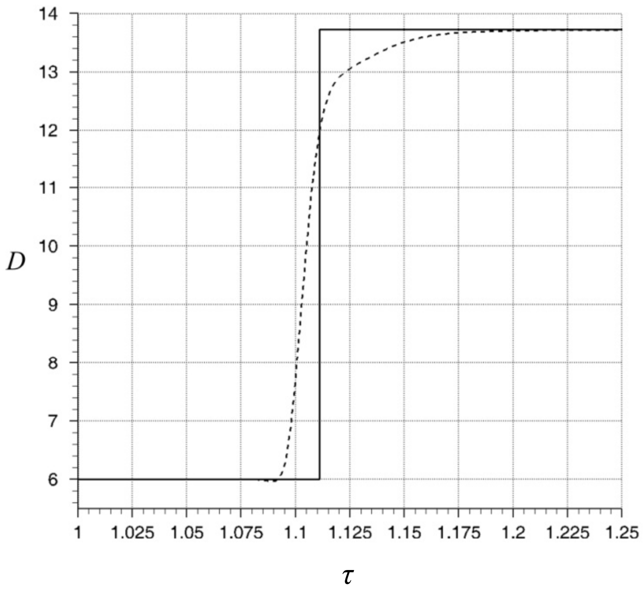
$$\frac{p_0^{n+1}}{P_0}=\frac{2\gamma}{\gamma+1}\left(M^{n+1}\right)^2-\frac{\gamma-1}{\gamma+1},\ \frac{\rho_0^{n+1}}{R_0}=\frac{(\gamma+1)\left(M^{n+1}\right)^2}{2+(\gamma-1)\left(M^{n+1}\right)^2},\ \frac{v_0^{n+1}}{C_0}=\frac{2}{\gamma+1}\frac{\left(M^{n+1}\right)^2-1}{M^{n+1}},\ Z_0^{n+1}=1.$$

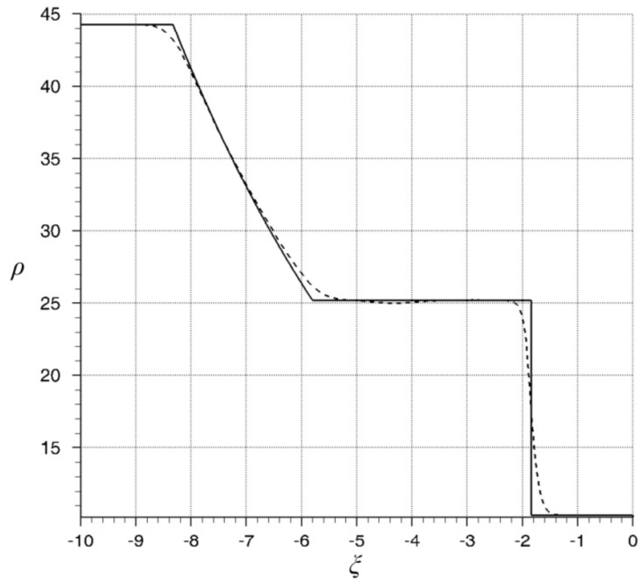
- Variables p_*^n, p_*^{n-1}, v_*^n, v_*^{n-1} are calculated using quadratic interpolation procedure.

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

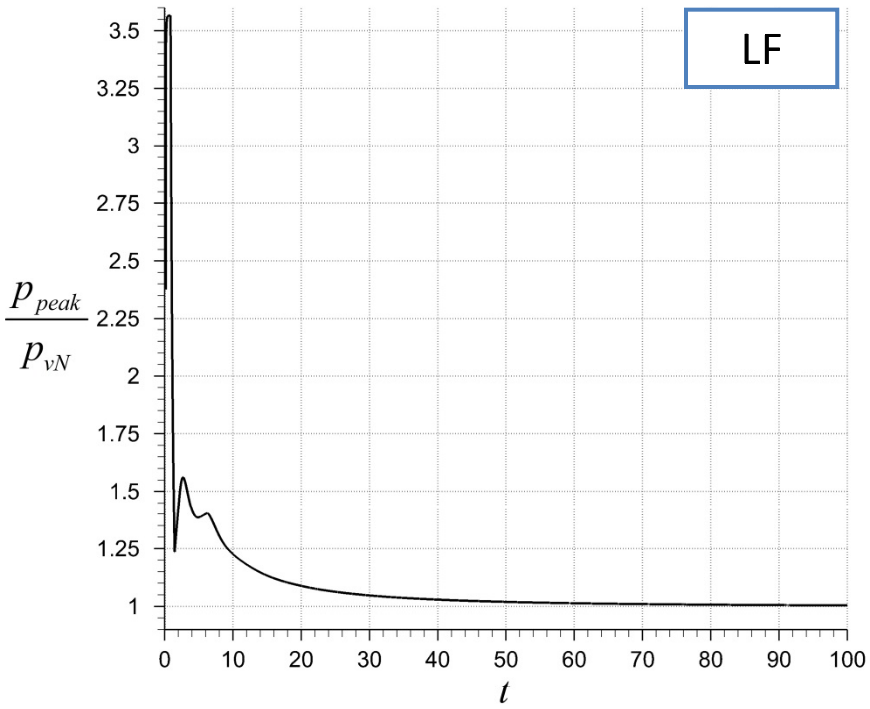


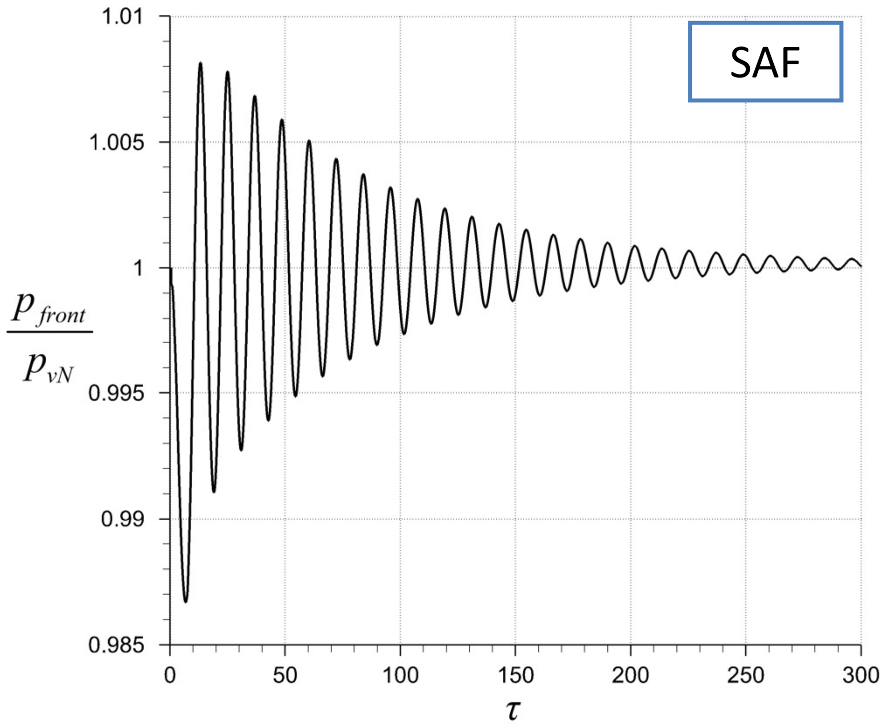




Stable regime

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



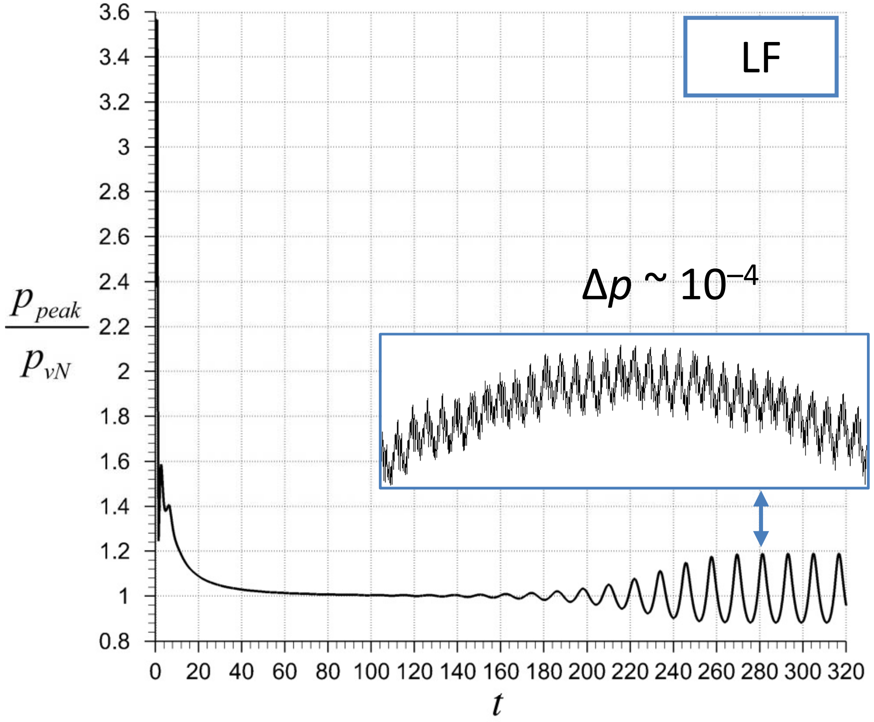


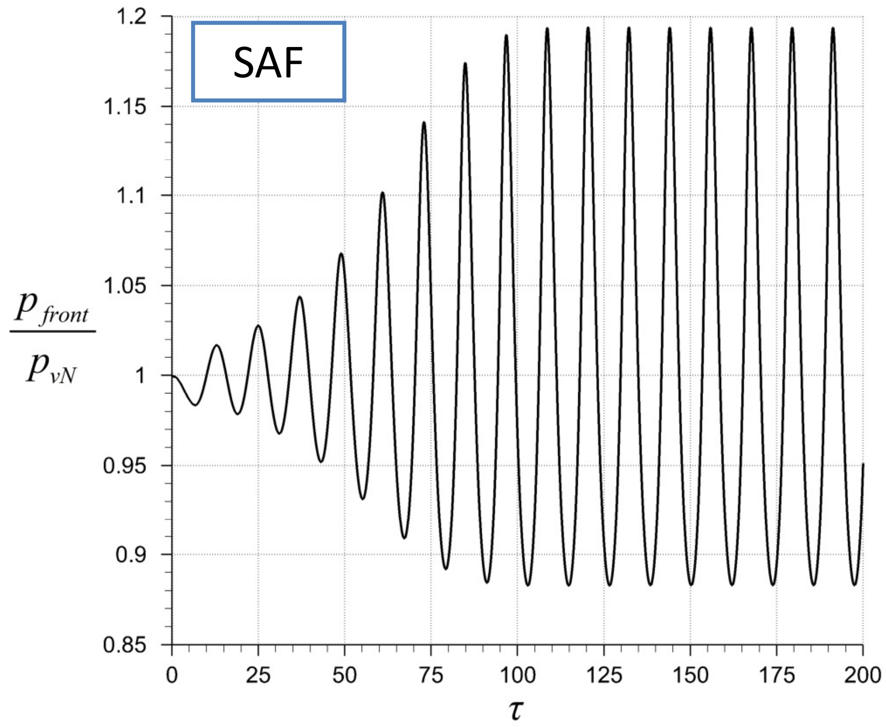
$$\left.\begin{array}{l} N_1 = 4000,\ \Delta_1 = \left| p_{front}^{calc1} / p_{vN} - 1.0 \right| \approx 0.000150 \\ N_1 = 2000,\ \Delta_2 = \left| p_{front}^{calc2} / p_{vN} - 1.0 \right| \approx 0.000495 \end{array}\right\}$$

$$\left| p_{front}^{calc} / p_{vN} - 1.0 \right| \sim Ch^k \qquad k \approx \frac{\ln(\Delta_2 / \Delta_1)}{\ln 2} \approx 1.72$$

Weakly unstable regime (1)

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



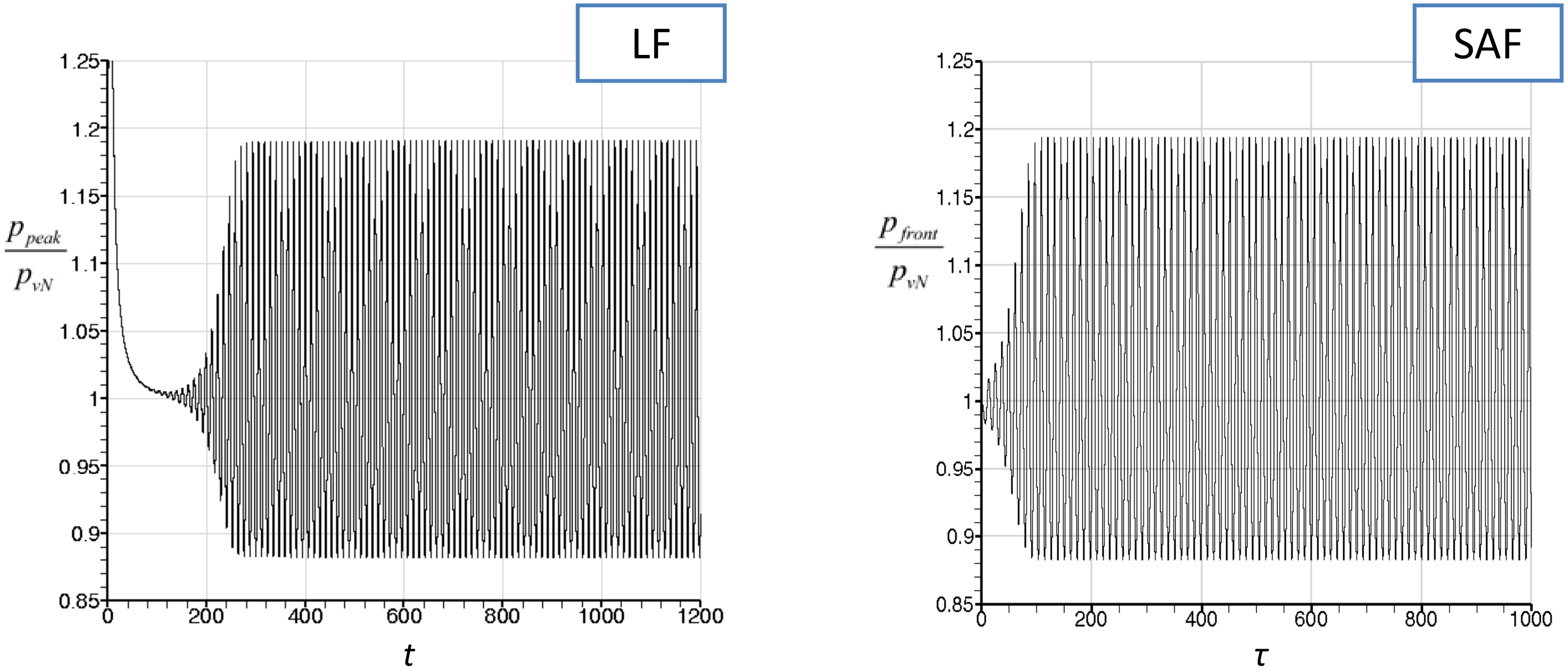


$T_{LF} = 11.79$ $T_{LIN} = 12.11$ $T_{SAF} = 11.85$

Lee H.I., Stewart D.S. Calculation of linear detonation instability: one-dimensional instability of plane detonation // Journal of Fluid Mechanics. 1990. V. 216. P. 103–132.

Weakly unstable regime (2)

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



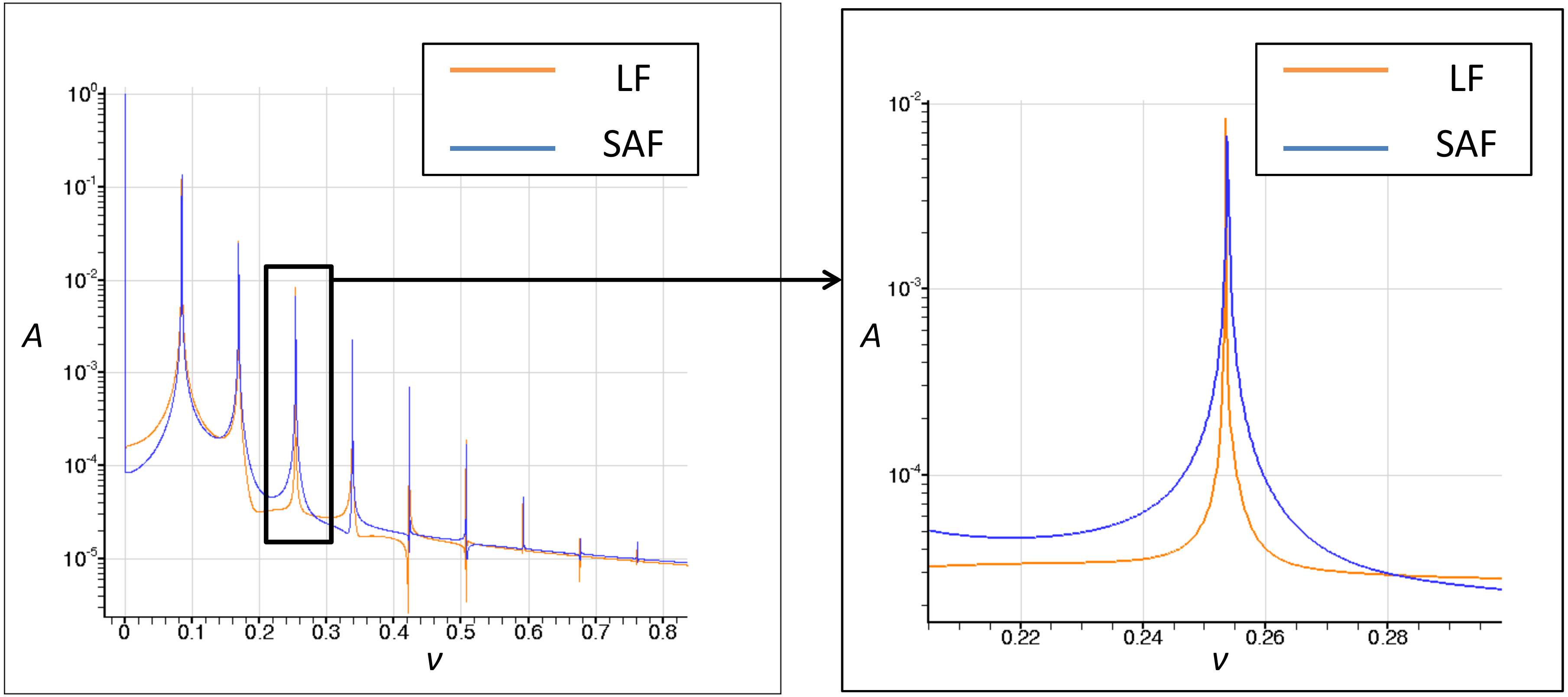
Long term numerical research

Weakly unstable regime (3)

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

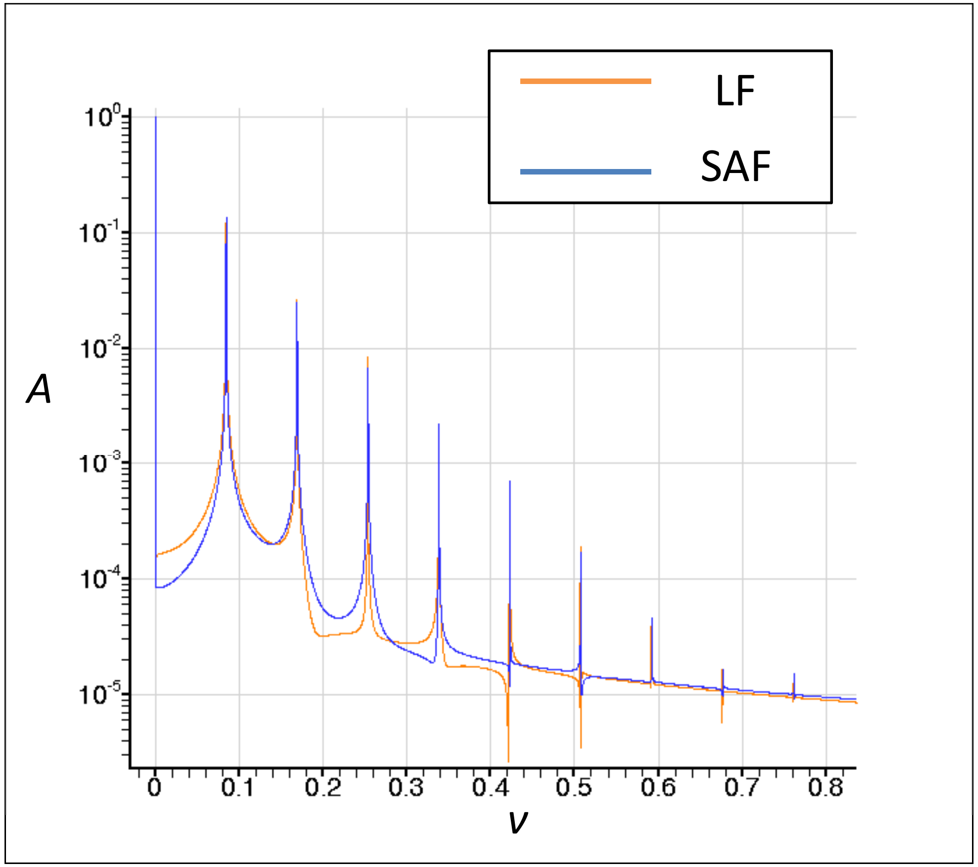
Fourier spectral analysis (5000 units of time)

$$\frac{\mathrm{p}}{\mathrm{p}_{\mathrm{vN}}} = \sum_{k=0}^{\infty} A_k \cdot \cos\left(2\pi \nu_k t\right)$$



Weakly unstable regime (4)

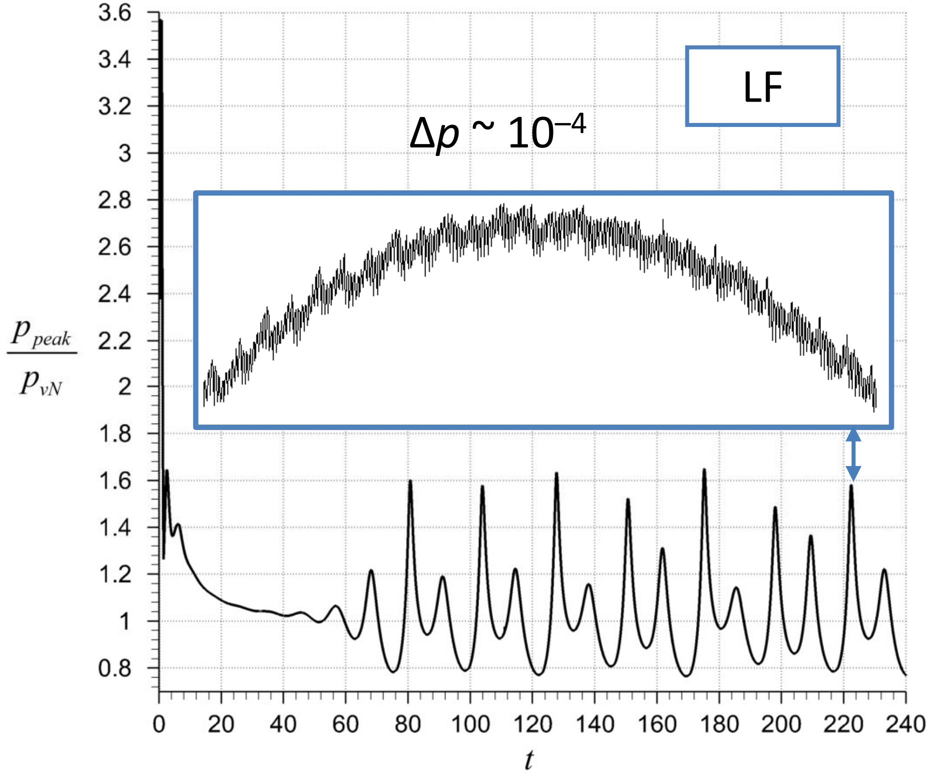
- Fourier spectra of two statements demonstrate similar values of peak frequencies

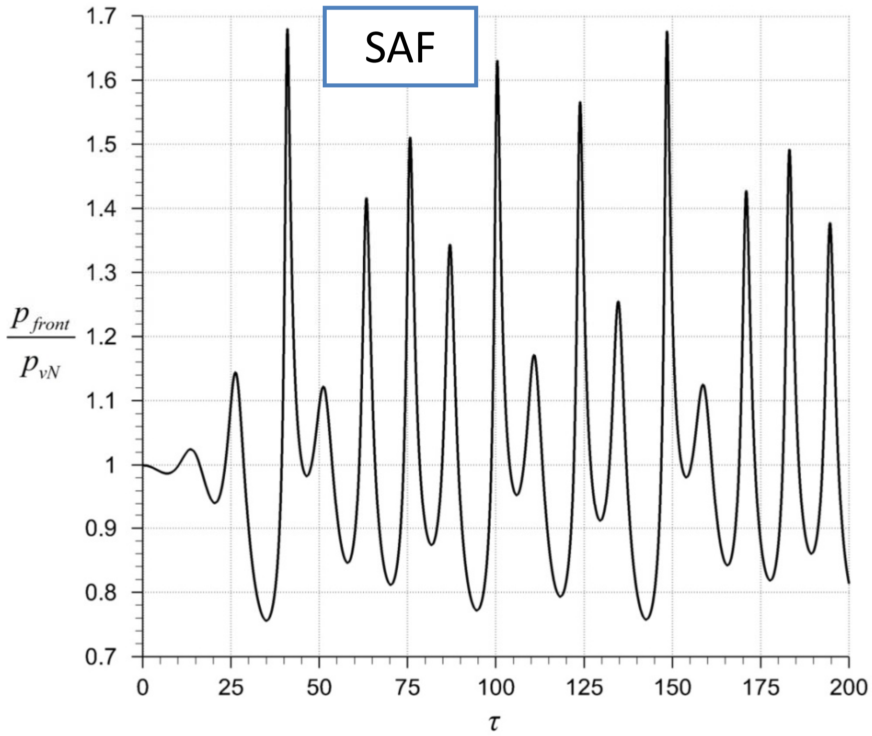


Peak	ν (LF)	ν (SAF)
0	0	0
1	0.08442	0.08464
2	0.16905	0.16929
3	0.25347	0.2537
4	0.33789	0.33834
5	0.42252	0.42299
6	0.50694	0.50764
7	0.59136	0.59228
8	0.67578	0.67693
9	0.76041	0.76133

Irregular regime (1)

E = 28, *Q* = 50, *γ* = 1.2, Δ*x* = 2.5·10^{-3}





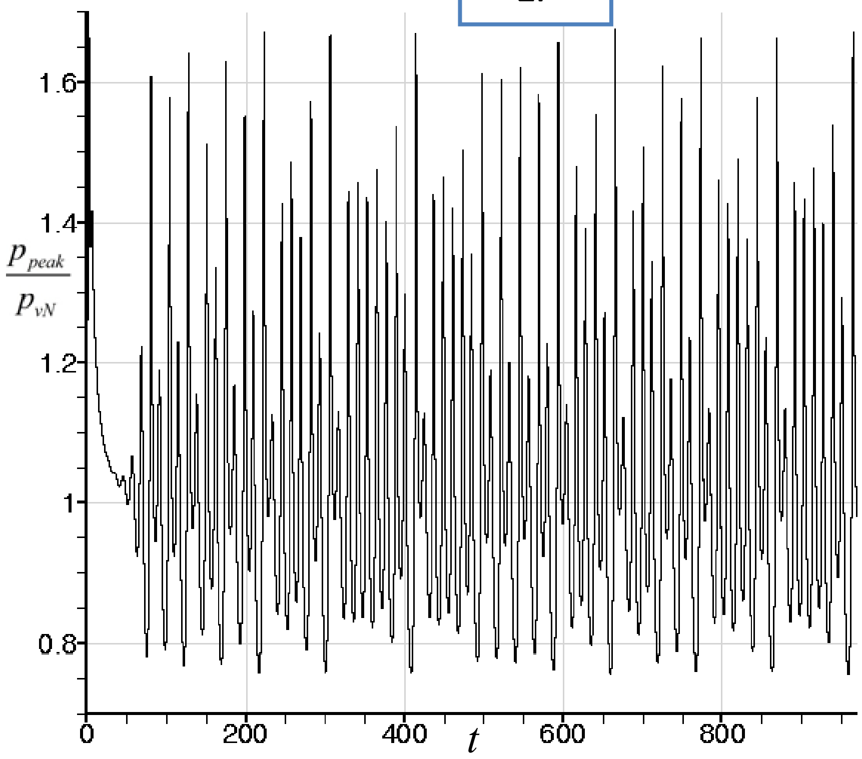
$$\frac{p_{\max}^{LF}}{p_{\min}^{LF}} = \frac{1.65}{0.76}$$

$$\frac{p_{\max}^{SAF}}{p_{\min}^{SAF}} = \frac{1.68}{0.76}.$$

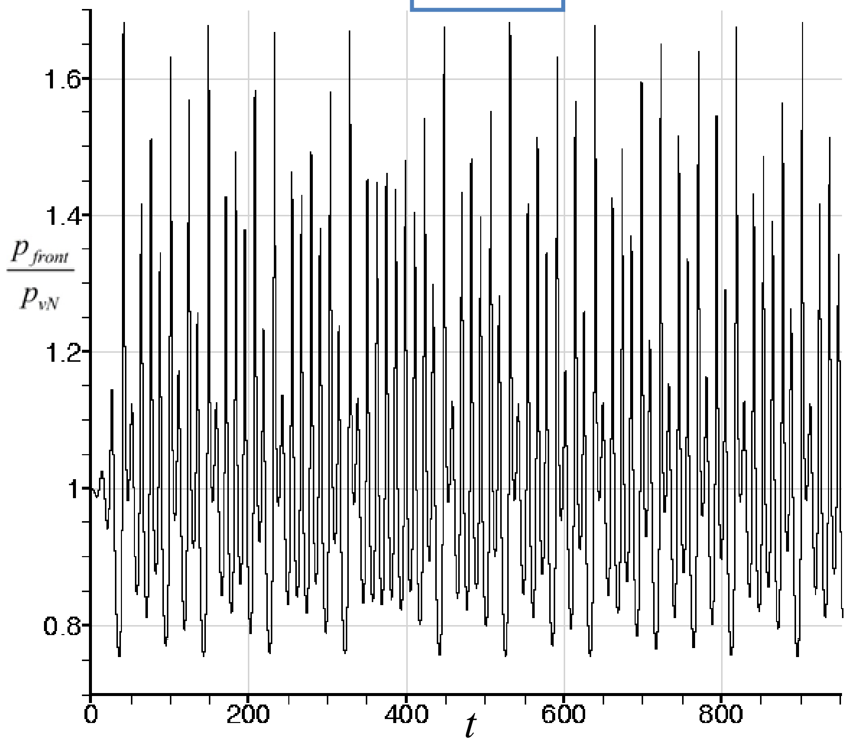
Irregular regime (2)

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

LF



SAF



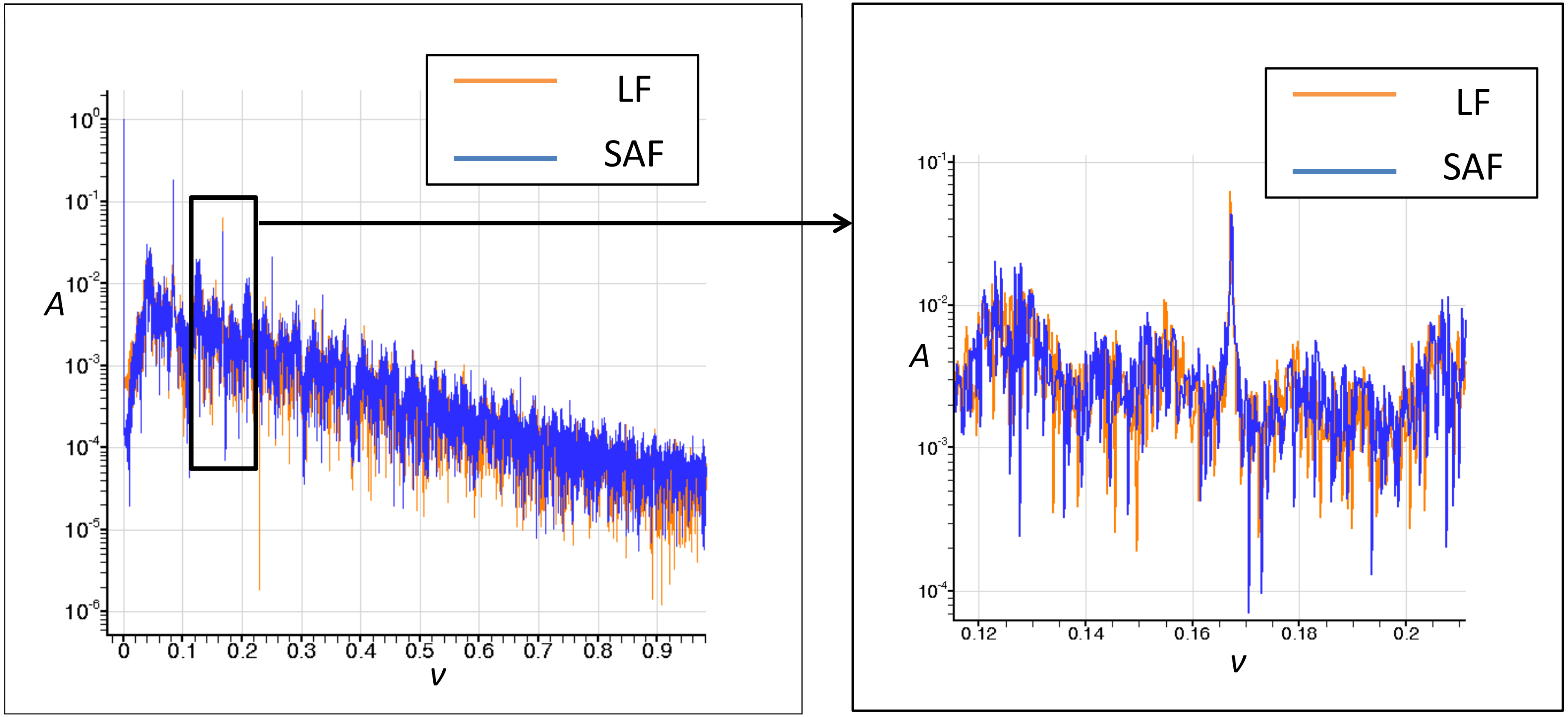
Long term numerical research

Irregular regime (3)

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

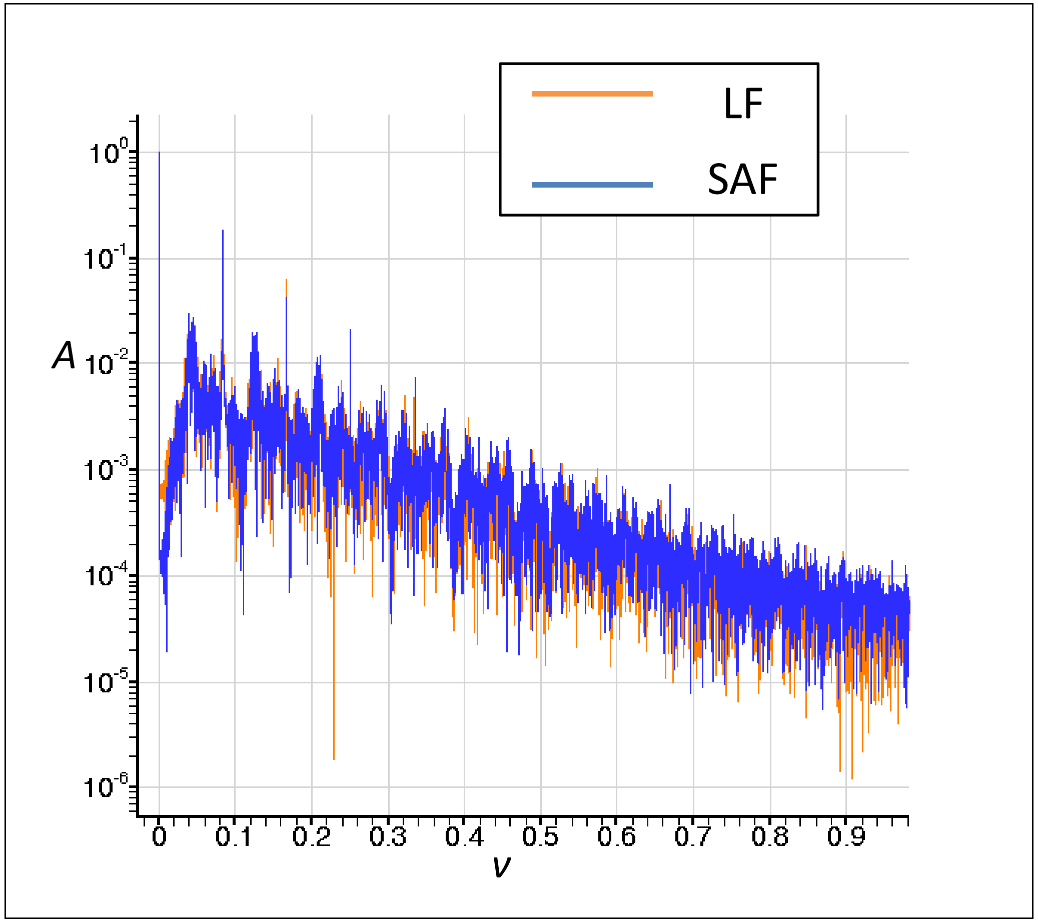
Fourier spectral analysis (5000 units of time)

$$\frac{p}{p_{vN}} = \sum_{k=0}^{\infty} A_k \cdot \cos\left(2\pi \nu_k t\right)$$



Irregular regime (4)

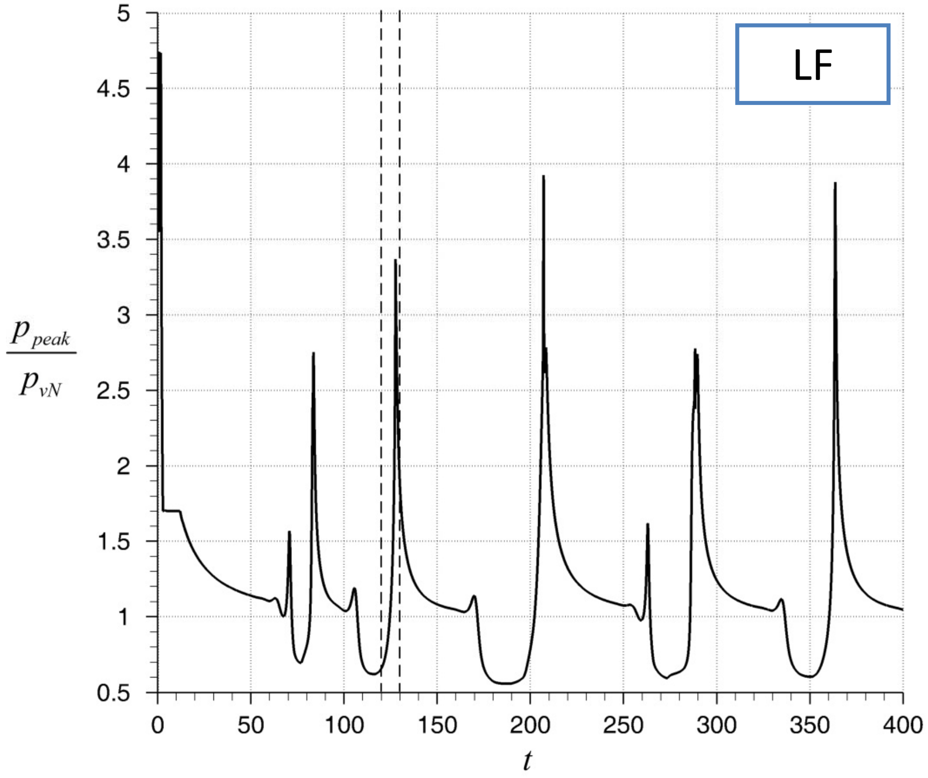
- Fourier spectra of two statements demonstrate similar values of peak frequencies

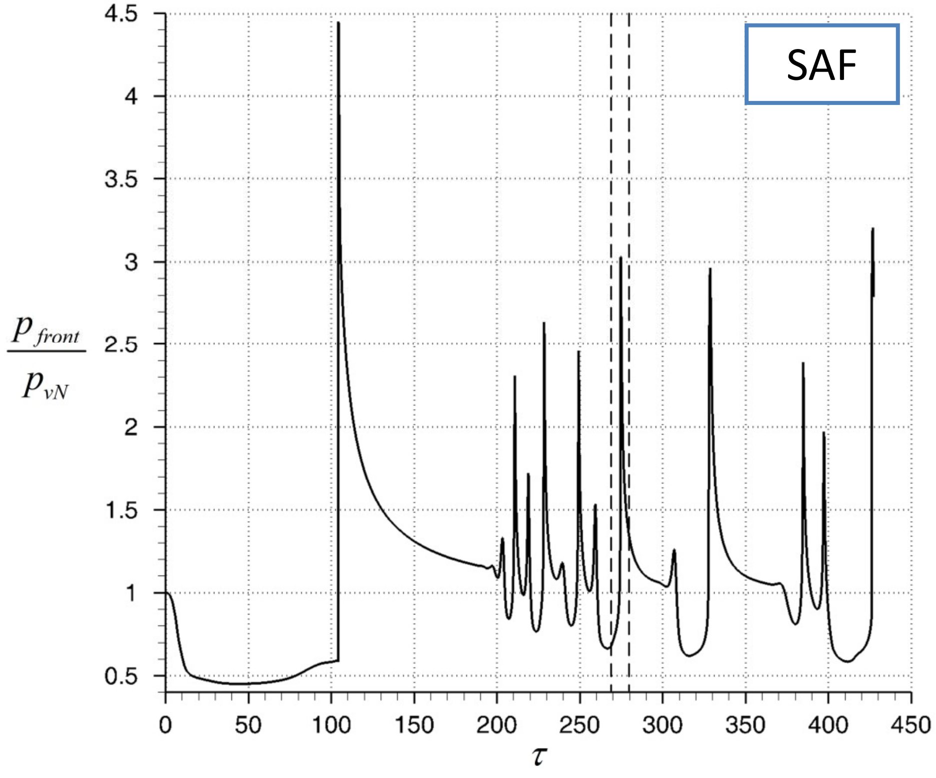


Peak	ν (LF)	ν (SAF)
0	0	0
1	0.08365	0.08371
2	0.16709	0.16721
3	0.25074	0.25093
4	0.33418	0.33464

Strongly-unstable regime (1)

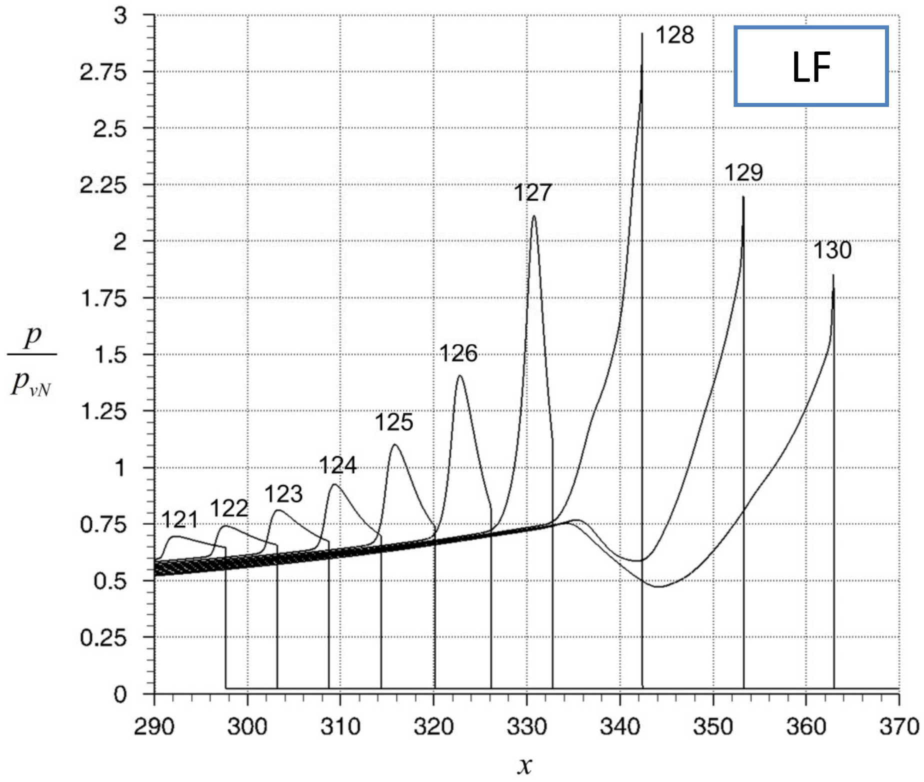
$E = 35, Q = 50, \gamma = 1.2, \Delta x = 3.75 \cdot 10^{-3}$

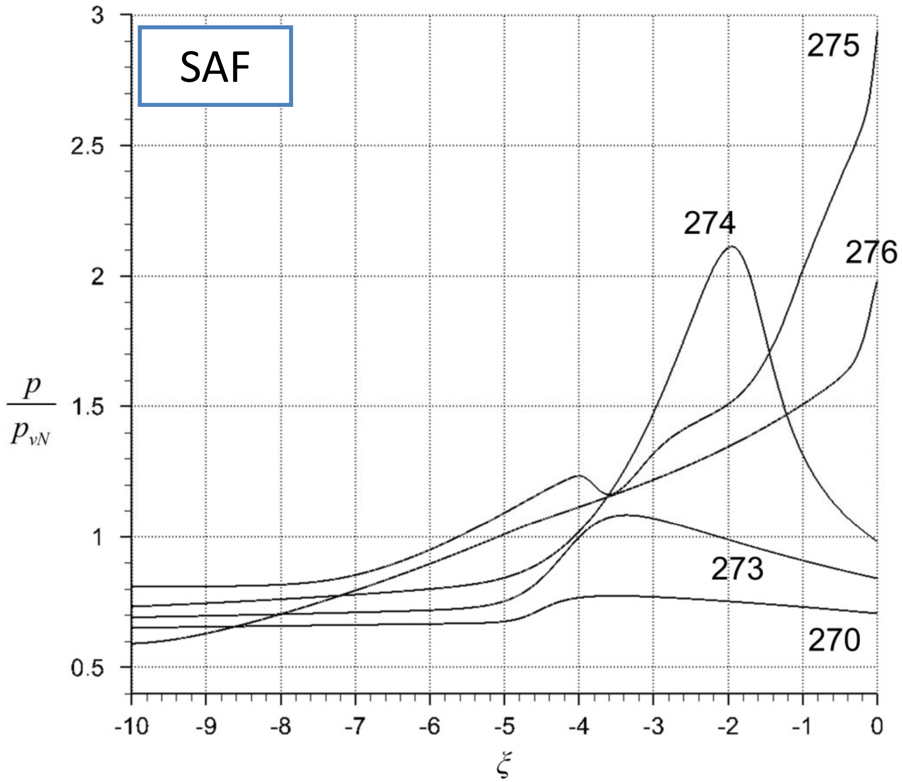




Strongly-unstable regime (2)

$E = 35$, $Q = 50$, $\gamma = 1.2$, $\Delta x = 3.75\cdot10^{-3}$





Conclusion

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.

Publications

1. Лопато, А.И., Уткин, П.С. Математическое моделирование пульсирующей волны детонации с использованием ENO-схем различных порядков аппроксимации // Компьютерные исследования и моделирование. – 2014. – Т. 6, № 5. – С. 643 – 653.
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 волны // Математическое моделирование. – 2016. – Т. 28, № 2. – С. 133 – 145.

   Lopato, A.I., Utkin, P.S. Two approaches to the mathematical modeling of detonation wave // Mathematical Models and Computer Simulations. – 2016. – V. 8, No. 5. – P. 585 – 594.
4. Лопато, А.И., Уткин, П.С. Детальное математическое моделирование пульсирующей детонационной волны в системе координат, связанной с лидирующим скачком // Журнал вычислительной математики и математической физики. – 2016. – Т. 56, № 5. – С. 856 – 868.

   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. **Lopato, A.I., Utkin, P.S. 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).**