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A variational approach to the shock structure problem

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Abstract

A variational approach to the shock structure problem is proposed. The set of governing equations, consisted of n first-order ordinary differential equations accompanied with $2n$ boundary conditions at $\pm\infty$, is put into variational form by means of least-squares method. The corresponding variational principle is adjusted for application of Ritz method. This direct method is used for construction of approximate analytical solutions to the shock structure problem and derivation of the estimates for the shock thickness. General procedure is applied to the study of Burgers' equation and equations of gas dynamics.

Key words: shock waves, variational principle, least-squares method, Ritz method.

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1 Introduction

Shock waves are discontinuous solutions of the systems of conservations laws localized on the singular surface ϕ - the wave front. In the case of one space dimension conservation laws could be expressed as:

$$\partial_t \mathbf{F}^0(\mathbf{u}) + \partial_x \mathbf{F}(\mathbf{u}) = \mathbf{0}, \tag{1}$$

where $\mathbf{F}^0$ and $\mathbf{F}$ are $n-$vectors of densities and fluxes of physical quantities, respectively, while $\mathbf{u}(x,t)$ is $n-$vector of field variables. Shock waves are then treated as singular surfaces $\phi(x,t) = x - st$ traveling with speed s and carrying jumps of field variables determined by Rankine-Hugoniot equations:

$$-s\left[\mathbf{F}^0(\mathbf{u})\right] + \left[\mathbf{F}(\mathbf{u})\right] = \mathbf{0}. \tag{2}$$

Brackets $[\mathbf{\Psi}] = \mathbf{\Psi}_1 - \mathbf{\Psi}_0$ are used to denote the jump of the quantity $\mathbf{\Psi}$ across the wave front, $\mathbf{\Psi}_0$ and $\mathbf{\Psi}_1$ being its values in front and behind the shock, respectively. By solving equations (2) the state $\mathbf{u}_1$ behind the shock is determined in terms of the state $\mathbf{u}_0$ in front of it and the shock speed s.

In reality, when dissipative effects are taken into account, shocks are smoothed out into continuous solutions asymptotically joining the states $\mathbf{u}_0$ and $\mathbf{u}_1$, with steep gradients in the neighborhood of the front $\phi = x - st$. Thus, dissipation equips shock waves with the structure. Usually, it is driven by viscosity and heat conduction, in which case the system (1) becomes the system of balance laws:

$$\partial_t \mathbf{F}^0(\mathbf{u}) + \partial_x \mathbf{F}(\mathbf{u}) = \mu \partial_x \left(\mathbf{B}(\mathbf{u}) \partial_x \mathbf{u}\right), \tag{3}$$

with $\mathbf{B}(\mathbf{u})$ being $n \times n-$matrix, or by relaxation when (1) transforms into a balance laws system with local source terms:

$$\partial_t \mathbf{F}^0(\mathbf{u}) + \partial_x \mathbf{F}(\mathbf{u}) = \frac{1}{\varepsilon} \mathbf{P}(\mathbf{u}). \tag{4}$$

In either case systems of balance laws can be transformed using traveling wave ansatz $\mathbf{u}(x,t) = \mathbf{v}(x-st) = \mathbf{v}(\xi)$, $\xi = x - st$, and reduced to the system of n ordinary differential equations:

$$\mathbf{v}' = \mathbf{f}(\mathbf{v}); \qquad -\infty < \xi < \infty, \tag{5}$$

where $(\,)' = d(\,)/d\xi$, accompanied with appropriate boundary conditions:

$$\lim_{\xi\to-\infty} \mathbf{v}(\xi) = \mathbf{u}_1, \qquad \lim_{\xi\to\infty} \mathbf{v}(\xi) = \mathbf{u}_0. \tag{6}$$

Since $\mathbf{u}_0$ and $\mathbf{u}_1$ are treated as equilibrium states, (6) can be replaced by an equivalent condition:

$$\lim_{\xi\to\pm\infty} \mathbf{v}'(\xi) = 0. \tag{7}$$

Boundary conditions (6) and (7) give rise to equations:

$$\mathbf{f}(\mathbf{u}_0) = \mathbf{0} \quad \text{and} \quad \mathbf{f}(\mathbf{u}_1) = \mathbf{0}, \tag{8}$$

which are equivalent to Rankine-Hugoniot equations (2).

Solution $\mathbf{v}(\xi)$ of the system (5) which satisfies boundary conditions (6) or (7) determines the shock structure (shock profile), also called viscous or relaxation profile emphasizing the mechanism of dissipation. It is a heteroclinic orbit in $n-$dimensional state space asymptotically connecting equilibrium states $\mathbf{u}_0$ and $\mathbf{u}_1$. This problem is over-determined in the sense that n first-order ODE's (5) are adjoined with $2n$ boundary conditions (6). Except in few particular cases, like Burgers' equation, shock structure cannot be determined in closed analytical form. Therefore, boundary-value problem (5)-(6) used to be solved approximately, either by perturbation techniques, motivated by the fact that μ in (3) and ε in (4) are small parameters, or by numerical integration.

The goal of this study is to develop a procedure for derivation of approximate analytical solutions of the shock structure problem

(5)-(6), or (5)-(7). It will be based upon least-squares method used in conjunction with the Ritz direct method of calculus of variations. This procedure is advantageous with respect to techniques mentioned earlier due to its simplicity, good results even with simple profiles and possibility for analytical study of the shock thickness - a parameter of great importance in the analysis of shock waves. In the next section a proper variational formulation of the problem will be given. In Section 3 it will be adjusted for application of the Ritz method. Finally, the proposed procedure will be tested in the shock structure analysis of Burgers' equation (Section 4) and gas dynamic equations (Section 5).

2 Variational formulation

Let us analyze the system of ODE's (5) with boundary conditions (7). In order to put this boundary-value problem into variational setup the following variational problem will be formulated:

$$J(\mathbf{V}) = \int_{-\infty}^{\infty} \left(\mathbf{V}' - \mathbf{f}(\mathbf{V})\right)^2 d\xi \to \min, \tag{9}$$

where $\mathbf{V}(\xi)$ is $n-$vector function from the set of admissible functions:

$$D = \left\{ \mathbf{V}(\xi) : \mathbf{V}(\xi) \in C^1(\mathbb{R}, \mathbb{R}^n); \lim_{\xi \to -\infty} \mathbf{V}'(\xi) = \lim_{\xi \to \infty} \mathbf{V}'(\xi) = \mathbf{0} \right\}. \tag{10}$$

It is obvious that $\min_{\mathbf{V}(\xi) \in D} J(\mathbf{V}) = 0$, if such a minimizer exists. Also, every $\mathbf{V}(\xi) \in D$ satisfies boundary conditions (7).

Proposition 2.1 *Functional (9) attains its minimum on the solution* $\mathbf{v}(\xi)$ *of the boundary-value problem (5),(7). Boundary conditions (8) appear as a consequence of transversality conditions of variational problem (9).*

Proof: First part of the proposition is trivial consequence of the fact that functional (9) ought to minimize the square of the differential system (5). If $\mathbf{v}(\xi)$ solves (5) and satisfies boundary conditions (7), then $\mathbf{v}(\xi) \in D$ and $J(\mathbf{v}) = 0$ as desired.

From the necessary condition of extremum, $\delta J(\mathbf{v}, \mathbf{h}) = 0$, where $\mathbf{h} = \mathbf{V} - \mathbf{v}$, one obtains Euler-Lagrange equations and transversality condition:

$$(\mathbf{v}' - \mathbf{f}(\mathbf{v})) \cdot \mathbf{h}|_{-\infty}^{\infty} = 0.$$

By the choice of set D we have $\mathbf{v}'(\xi) \to \mathbf{0}$ and $\mathbf{h}(\xi)$ arbitrary at infinity. This leads to:

$$\lim_{\xi \to \pm\infty} \mathbf{f}(\mathbf{v}(\xi)) = \mathbf{0}.$$

It may be concluded that boundary states $\mathbf{u}_0$ at ∞ and $\mathbf{u}_1$ at $-\infty$ are equilibrium states - stationary points, thus proving the second part of the proposition.

Remark 1. If $\mathbf{v}(\xi)$ is $C^2(\mathbb{R}, \mathbb{R}^n)$ solution of (5),(7), then it identically satisfies Euler-Lagrange equations $(d/d\xi)(\partial L/\partial \mathbf{v}') - \partial L/\partial \mathbf{v} = \mathbf{0}$ of variational problem (9) with Lagrangian function:

$$L(\mathbf{V}, \mathbf{V}') = (\mathbf{V}' - \mathbf{f}(\mathbf{V}))^2 . \tag{11}$$

This conclusion can be drawn directly from the following form of Euler-Lagrange equations:

$$\frac{d}{d\xi} (\mathbf{v}' - \mathbf{f}(\mathbf{v})) + (\mathbf{v}' - \mathbf{f}(\mathbf{v})) \frac{\partial \mathbf{f}(\mathbf{v})}{\partial \mathbf{v}} = \mathbf{0}. \tag{12}$$

Moreover, an explicit form of (12) reads:

$$\mathbf{v}'' = \frac{\partial \mathbf{f}(\mathbf{v})}{\partial \mathbf{v}} \mathbf{f}(\mathbf{v}), \tag{13}$$

representing the derivative of the system (5) along its solution curve.

Remark 2. Proposition 2.1 and conclusions of previous remark remain unchanged even if the system (5) is non-autonomous, $\mathbf{f} = \mathbf{f}(\mathbf{v}, \xi)$. Only the structure of (13) is a bit different:

$$\mathbf{v}'' = \frac{\partial \mathbf{f}(\mathbf{v}, \xi)}{\partial \xi} + \frac{\partial \mathbf{f}(\mathbf{v}, \xi)}{\partial \mathbf{v}} \mathbf{f}(\mathbf{v}, \xi).$$

Remark 3. Right-hand side of the system (5) also depends on the shock speed s as a parameter, i.e. $\mathbf{f} = \mathbf{f}(\mathbf{v}, s)$. This has to be taken into account because equilibrium states could depend on s. In particular, one can obtain $\mathbf{u}_1 = \mathbf{u}_1(\mathbf{u}_0, s)$ either as solution of Rankine-Hugoniot equations (2) or boundary conditions (8). Furthermore, shock waves and corresponding profiles exist only for certain ranges of the value of shock speed. This issue is very important and there exist several selection rules for physically admissible shocks (Lax condition, entropy criterion, Liu condition). A detailed account on this problem could be found in [5] and [11].

3 The direct method

Variational principle (9) formulated on the set (10) gives an appropriate setup for the shock structure problem (5),(7). Nevertheless, infinite domain of independent variable ξ could cause difficulties either in basic or in variational formulation. In numerical approach to (5),(7) this problem could be overcome by elimination of independent variable and reduction of order of the system by one. This appeared to be a fruitful idea since (5) is an autonomous system and the region of the state space where heteroclinic orbit appears is bounded. Another possibility calls for enlargement of the finite domain of integration $\xi \in [\xi_0, \xi_1]$ until desired accuracy is reached. It is assumed that $\mathbf{v}'(\xi) \to \mathbf{0}$ as ξ tends to the endpoints. Here, a variant of the latter approach will be adopted in order to facilitate easier application of the direct method.

Instead of using set D of admissible functions, we shall search for the solution of variational problem (9) in the subset $\tilde{D} \subset D$ defined as follows:

$$\tilde{D} = \left\{ \mathbf{V}(\xi) : \mathbf{V}(\xi) \in C^1(\mathbb{R}, \mathbb{R}^n);\ \lim_{\xi \to \xi_0^+} \mathbf{V}'(\xi) = \lim_{\xi \to \xi_1^-} \mathbf{V}'(\xi) = \mathbf{0}; \mathbf{V}'(\xi) \equiv \mathbf{0}, \xi \in \mathbb{R} \setminus (\xi_0, \xi_1) \right\}. \tag{14}$$

Functions $\mathbf{V}(\xi) \in \tilde{D}$ reach equilibrium states at the endpoints of the interval $[\xi_0, \xi_1]$ and remain constant outside. The question of existence of the minimizer $\tilde{\mathbf{v}}(\xi) \in \tilde{D}$, $J(\tilde{\mathbf{v}}) = \min_{\mathbf{V}(\xi) \in \tilde{D}} J(\mathbf{V})$ will not be tackled here. The set (14) will serve only as a source of trial functions for the Ritz method.

In direct methods infinite dimensional problems are replaced by finite dimensional ones when approximate solutions are supposed in the form:

$$\mathbf{V} = \mathbf{V}(\xi, a_1, \ldots, a_n) \in \tilde{D}. \tag{15}$$

Constants a_i, $i = 1, \ldots, n$, are determined in the course of minimization of the functional (9) which now reads:

$$J(a_i) = \int_{-\infty}^{\infty} \mathbf{R}^2(\xi, a_i) d\xi, \tag{16}$$

where:

$$\mathbf{R}(\xi, a_i) = \mathbf{V}'(\xi, a_i) - \mathbf{f}(\mathbf{V}(\xi, a_i)),$$

represents the residual evaluated on approximate solution (15). Minimization with respect to a_i leads to the following necessary conditions for the extremum:

$$\frac{\partial J}{\partial a_i} = \int_{-\infty}^{\infty} 2\mathbf{R}(\xi, a_i) \cdot \frac{\partial \mathbf{R}(\xi, a_i)}{\partial a_i} \, d\xi = 0. \tag{17}$$

Given in this form, lest-squares method appears to be the special case of the method of weighted residuals, see [6].

Direct methods were successfully applied to irreversible and non-linear physical processes like heat transfer and boundary-layer flow in fluid mechanics. One may see a lot of examples in books of Biot [3], Finlayson [6], Vujanovic and Jones [12] and references cited therein. Their common characteristic is disobedience of some rules of the classical calculus of variations since governing equations cannot be derived from variational principle in a usual way. On the other hand, application of the least-squares method was criticized due to complicated equations it produces [6] and basically mathematical rather then physical origin [3].

Variational principle (9) applied to the shock structure problem (5),(7) provides a proper variational formulation and seems to be a good basis for the application of direct methods. Moreover, using approximate analytical solutions obtained in such a way one may calculate an estimate for one the most important quantities in the shock structure problem - shock thickness δ_S. Usually, it is defined as:

$$\delta_S = \left| \frac{v_{k1} - v_{k0}}{\max(dv_k/d\xi)} \right|, \tag{18}$$

where v_k is a particular component of the vector $\mathbf{v}$ of field variables, v_{k0} and v_{k1} being its equilibrium values. This will also be one of the outcomes of the present study.

4 Burgers' equation

As a first application of the procedure developed in previous sections we shall analyze approximate solution of the shock structure problem for Burgers' equation:

$$\partial_t u + \partial_x \left(\frac{1}{2} u^2 \right) = \nu \partial_{xx}^2 u. \tag{19}$$

It is the simplest example of the model which possesses both nonlinear propagation effects, leading to shock waves, and diffusion-like dissipative effects. By means of the Hopf-Cole transformation (19) can be reduced to linear heat equation and thus solved in closed form. This and many other remarkable features of Burgers' equation reader could find in the book of Whitham [14].

4.1 Shock structure problem and exact solution

Rankine-Hugoniot equation for (19), which reads $-s[u] + [u^2/2] = 0$, $[u] = u_1 - u_0$, has two solutions, one of them being:

$$s = \frac{1}{2} (u_1 + u_0) \quad \Leftrightarrow \quad u_1 = 2s - u_0, \tag{20}$$

while the other one is trivial, $u_1 = u_0$. Shock waves, determined by non-trivial solution (20), are admissible for $u_0 < s < u_1$. Differential equation for the viscous profile, obtained by the use of traveling wave ansatz $u(x,t) = v(x - st) = v(\xi)$ becomes:

$$v' = -\frac{1}{\nu}(v - u_0) \left(s - \frac{1}{2}(v + u_0) \right), \tag{21}$$

or equivalently:

$$v' = -\frac{1}{2\nu}(v - u_0)(u_1 - v). \tag{22}$$

It is obvious that boundary conditions (7) at infinity, i.e.:

$$\lim_{\xi \to \pm\infty} v'(\xi) = 0, \tag{23}$$

imply $v = u_0$ and $v = u_1$ are equilibrium states - stationary points of (22). Exact solution of boundary-value problem (22)-(23) is:

$$v(\xi) = u_0 + \frac{u_1 - u_0}{1 + \exp\left\{(u_1 - u_0)\frac{\xi}{2\nu}\right\}}. \tag{24}$$

To achieve as much generality as possible boundary-value problem (22)-(23) will be put into dimensionless form using following dimensionless quantities:

$$\hat{v} = \frac{v - u_0}{u_1 - u_0}; \qquad \hat{\xi} = \frac{u_1 - u_0}{\nu}\,\xi. \tag{25}$$

In such a way we arrive to:

$$\frac{d\hat{v}}{d\hat{\xi}} = -\frac{1}{2}\hat{v}(1 - \hat{v}); \qquad \lim_{\hat{\xi} \to \pm\infty} \frac{d\hat{v}}{d\hat{\xi}}(\hat{\xi}) = 0, \tag{26}$$

whose exact solution - dimensionless counterpart of (24) - has the following form:

$$\hat{v}(\hat{\xi}) = \frac{1}{1 + \exp\left(\frac{\hat{\xi}}{2}\right)}, \tag{27}$$

Equilibrium states and shock speed thus become $\hat{u}_0 = 0$, $\hat{u}_1 = 1$ and $\hat{s} = 1/2$.

4.2 Variational approximation

Variational principle (9) applied to boundary-value problem (26) reads:

$$J(\hat{V}) = \int_{-\infty}^{\infty} \left(2\frac{d\hat{V}}{d\hat{\xi}} + \hat{V}(1 - \hat{V})\right)^2 d\hat{\xi} \to \min\,. \tag{28}$$

Approximate solution will be searched for in the following subset of admissible functions:

$$\tilde{D} = \left\{ \hat{V}(\hat{\xi}) : \hat{V}(\hat{\xi}) \in C^1(\mathbb{R}); \lim_{\hat{\xi} \to -\hat{a}^+} \frac{d\hat{V}}{d\hat{\xi}}(\hat{\xi}) = \lim_{\hat{\xi} \to \hat{a}^-} \frac{d\hat{V}}{d\hat{\xi}}(\hat{\xi}) = 0; \frac{d\hat{V}}{d\hat{\xi}}(\hat{\xi}) \equiv 0, \hat{\xi} \in \mathbb{R} \setminus (-\hat{a}, \hat{a}) \right\}. \tag{29}$$

Symmetric interval $(-\hat{a}, \hat{a})$ in $\tilde{D}$ is motivated by the symmetry properties of exact solution (27). Corresponding endpoints of the original interval $(-a, a)$ are determined by relation $a = \nu \hat{a}/(u_1 - u_0)$.

As a first approximation of (27) let us suppose the solution in the form:

$$\hat{v}^{(1)}(\hat{\xi}) = \begin{cases} 1, & \hat{\xi} \in (-\infty, -\hat{a}], \\ a_0 + a_1\hat{\xi} + a_2\hat{\xi}^2 + a_3\hat{\xi}^3, & \hat{\xi} \in (-\hat{a}, \hat{a}), \\ 0, & \hat{\xi} \in [\hat{a}, \infty) \end{cases}$$

In order to insure $\hat{v}^{(1)}(\hat{\xi}) \in \tilde{D}$ it has to satisfy boundary conditions:

$$\hat{v}(-\hat{a}) = 1; \quad \hat{v}(\hat{a}) = 0; \quad \frac{d\hat{v}}{d\hat{\xi}}(\pm\hat{a}) = 0, \tag{30}$$

In such a way first approximation is obtained in the form:

$$\hat{v}^{(1)}(\hat{\xi}) = \frac{1}{2} - \frac{3}{4}\frac{\hat{\xi}}{\hat{a}} + \frac{1}{4}\left(\frac{\hat{\xi}}{\hat{a}}\right)^3, \tag{31}$$

for $\hat{\xi} \in (-\hat{a}, \hat{a})$. Observe that the only adjustable parameter in (31) is $\hat{a}$ which will stretch the profile to obtain the best approximation with respect to (28). By putting $\hat{v}^{(1)}(\hat{\xi})$ into (28) a function of single independent variable $\hat{a}$ is obtained:

$$J(\hat{v}^{(1)}) = J(\hat{a}) = -\frac{2}{3} + \frac{12}{5\hat{a}} + \frac{243}{5005}\hat{a}. \tag{32}$$

In the spirit of the Ritz method we shall search for the stationary point of $J(\hat{a})$, i.e. $dJ/d\hat{a} = 0$, and obtain the result:

$$\hat{a} = (2/9)\sqrt{1001} \approx 7.031 \quad J^{(1)} = 0.016. \tag{33}$$

It can be seen that even such a poor profile like (31) gives a good approximation of exact solution (27).

We may improve the results just obtained by expanding the power-law approximation. The calculations could be simplified if we take into account symmetry properties of exact solution and drop all the terms of even degree. Therefore, non-constant part of second approximation could be assumed in the form $\hat{v}^{(2)}(\hat{\xi}) = a_0 + a_1\hat{\xi} + a_3\hat{\xi}^3 + a_5\hat{\xi}^5$. Profile which matches the boundary conditions (30) then reads:

$$\hat{v}^{(2)}(\hat{\xi}) = \frac{1}{2} + \left(\frac{-3}{4\,\hat{a}} + \hat{a}^4 a_5\right)\hat{\xi} + \left(\frac{1}{4\,\hat{a}^3} - 2\,\hat{a}^2 a_5\right)\hat{\xi}^3 + a_5\hat{\xi}^5. \tag{34}$$

Substitution of $\hat{v}^{(2)}(\hat{\xi})$ into (28) leads to the function:

$$\begin{aligned} J(\hat{v}^{(2)}) = J(\hat{a}, a_5) = &-\frac{2}{3} + \frac{12}{5\,\hat{a}} + \frac{243\,\hat{a}}{5005} - \frac{64\,\hat{a}^4 a_5}{35} + \frac{2176\,\hat{a}^6 a_5}{45045} \\ &+ \frac{1024\,\hat{a}^9 a_5^2}{315} + \frac{512\,\hat{a}^{11} a_5^2}{58905} - \frac{8192\,\hat{a}^{16} a_5^3}{373065} + \frac{65536\,\hat{a}^{21} a_5^4}{14549535}. \end{aligned} \tag{35}$$

Necessary conditions of extremum $\partial J/\partial\hat{a} = 0$, $\partial J/\partial a_5 = 0$ yield the following result:

$$\hat{a} = 8.456; \quad a_5 = -4.33 \times 10^{-6}; \quad J^{(2)} = 0.009. \tag{36}$$

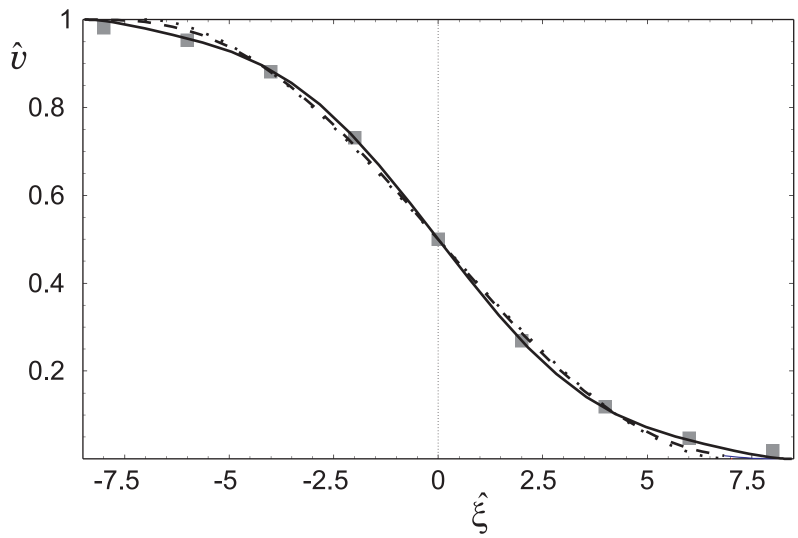

Figure 1: Exact and approximate solutions of Burgers' equation: $\hat{v}(\hat{\xi})$ - boxes, $\hat{v}^{(1)}(\hat{\xi})$ - dotted, $\hat{v}^{(2)}(\hat{\xi})$ - dashed, $\hat{v}^{(3)}(\hat{\xi})$ - solid

Value of the functional $J^{(2)} < J^{(1)}$ shows that this approximation is better than (31).

As a final test for our procedure a seventh-degree approximation will be assumed. Its non-constant part compatible with boundary conditions (30) has the form:

$$\begin{aligned} \hat{v}^{(3)}(\hat{\xi}) = \frac{1}{2} &+ \left(\frac{-3}{4\,\hat{a}} + \hat{a}^4 a_5 + 2\,\hat{a}^6 a_7\right)\hat{\xi} \\ &+ \left(\frac{1}{4\,\hat{a}^3} - 2\,\hat{a}^2 a_5 - 3\,\hat{a}^4 a_7\right)\hat{\xi}^3 + a_5\hat{\xi}^5 + a_7\hat{\xi}^7. \end{aligned} \tag{37}$$

Using this trial function (28) becomes $J(\hat{v}^{(3)}) = J(\hat{a}, a_5, a_7)$, whose form will be skipped for the sake of brevity. Necessary conditions of extremum $\partial J/\partial \hat{a} = 0$, $\partial J/\partial a_5 = 0$ and $\partial J/\partial a_7 = 0$ yield the result:

$$\hat{a} = 8.457; \quad a_5 = -2.62 \times 10^{-5}; \quad a_7 = 1.35 \times 10^{-7}; \quad J^{(3)} = 0.002. \tag{38}$$

Inspection of the values of the least-squares functional (28) shows that power-law approximations converge to exact solution (27).

Graphs of exact solution $\hat{v}(\hat{\xi})$ and approximate ones $\hat{v}^{(k)}(\hat{\xi})$, $k = 1, 2, 3$, shown in Figure 1., give an impression of the accuracy of solutions obtained via Ritz method. It can be seen that they converge to exact solution so that $\hat{v}^{(3)}(\hat{\xi})$ is almost indistinguishable from it.

Besides the value of (28), shock thickness could also be used for comparison of exact and approximate solutions. In dimensionless form it can be expressed as:

$$\hat{\delta} = \frac{\hat{u}_1 - \hat{u}_0}{\max |d\hat{u}/d\hat{\xi}|} = \frac{1}{\max |d\hat{u}/d\hat{\xi}|}.$$

Since $d\hat{u}/d\hat{\xi}$ reaches its maximum at $\hat{\xi} = 0$ for both exact and approximate solutions, it is easy to compare their values, $\hat{\delta}^{(E)}$ being the thickness of exact solution (27):

$$\hat{\delta}^{(1)} = 9.374; \quad \hat{\delta}^{(2)} = 9.021; \quad \hat{\delta}^{(3)} = 8.100; \quad \hat{\delta}^{(E)} = 8.0. \tag{39}$$

Once again one can observe convergence of approximate solutions to exact one. Moreover, dimensional shock thickness can be expressed as:

$$\delta = \frac{\nu}{u_1 - u_0} \hat{\delta},$$

and it is easy to see that it will increase with the increase of ν, which plays the role of viscosity, whereas the increase of shock strength $u_1 - u_0$ decreases the thickness.

5 Shock waves in gas dynamics

Another application will be concerned with the structure of shock waves in gas dynamics. Since this problem could be treated both from theoretical and experimental point of view, there is a lot of results providing either experimental data, or analysis of different models with a tentative of providing the range of their validity. Two basic theoretical approaches are continuum one, i.e. Navier-Stokes-Fourier model which comprises both viscosity and heat conduction effects, and kinetic theory, i.e. analytical or numerical solution of Boltzmann equation. Recently, there appeared yet another approach based upon extended thermodynamic theory, interesting because of the hyperbolic structure of governing equations and finite speeds of pulse propagation. Here, we shall seek for the approximate solutions of the shock structure equations obtained from Navier-Stokes-Fourier model.

Attempts to determine the validity of continuum approach to shock waves in fluids could be traced back to the paper of Becker [2] who obtained analytical solution of the shock structure equations although under physically unrealistic assumptions. Later on Gilbarg and Paolucci [7] gave the first qualitatively acceptable results based upon numerical solution of shock structure equations. Extended thermodynamic theory [8] gave another possibility of testing continuum approach to this problem. In the papers of Ruggeri [9], [10] and Weiss [13] one can find information about successes of this theory and obstacles that should have been avoided, major one being the breakdown of continuous solution when shock speed exceeds the highest characteristic speed of the governing system of equations. Finally, let us mention that valuable information about experimental results could be found in a paper of Alsmeyer [1]. He also reports that actually the best matching of theory and experiment have been obtained by Bird [4] through the application of Monte Carlo methods to the kinetic-theory model.

This review of previous work may be concluded with remark that there is a lack of analytical solutions, either exact or approximate, to the shock structure problem in gas dynamics. Therefore, it is worth trying to find such a solution which could provide simple but useful relations between important physical parameters.

5.1 Shock structure equations

Let us analyze one-dimensional balance laws of mass, momentum and energy for a monatomic gas:

$$\begin{aligned}
&\partial_t\rho + \partial_x(\rho v) = 0; \\
&\partial_t(\rho v) + \partial_x\left(\rho v^2 + p - \sigma\right) = 0; \\
&\partial_t\left(\rho e + \frac{1}{2}\rho v^2\right) + \partial_x\left\{\left(\rho e + \frac{1}{2}\rho v^2\right)v + pv - \sigma v + q\right\} = 0,
\end{aligned} \tag{40}$$

with usual notation: ρ - density, v - velocity, p - pressure, σ - $\langle 11\rangle$-component of stress deviator, e - internal energy and q - heat flux. These equations are adjoined with thermal and caloric equation of state:

$$p = \rho\frac{k}{m}T; \qquad e = \frac{3}{2}\frac{k}{m}T, \tag{41}$$

and Navier-Stokes and Fourier constitutive equations for stress and heat flux:

$$\sigma = \frac{4}{3}\mu\,\partial_x v; \qquad q = -\kappa\,\partial_x T. \tag{42}$$

Here we have: k - Boltzmann constant, m - atomic mass of a gas, μ - viscosity (combination of shear and compression one) and κ - thermal conductivity. Following Gilbarg and Paolucci [7] we shall assume that viscosity and thermal conductivity are temperature dependent:

$$\mu = \frac{1}{\alpha}\frac{k}{m}T^r; \quad \kappa = \frac{15}{4}\frac{k}{m}\mu. \tag{43}$$

where exponent r depends on the type of gas and factor α depends on the strength of intermolecular forces.

By assuming the solution of (40) in a traveling wave form, $\mathbf{u}(x,t) = \mathbf{v}(x - st) = \mathbf{v}(\xi)$, $\mathbf{u} = (\rho, v, T)^T$, one obtains the following set of equations:

$$\begin{aligned} &\frac{d}{d\xi}(\rho u) = 0; \\ &\frac{d}{d\xi}\left(\rho u^2 + p - \sigma\right) = 0; \\ &\frac{d}{d\xi}\left(\rho u^3 + 5pu - 2\sigma u + 2q\right) = 0, \end{aligned} \tag{44}$$

where $u = v - s$ is relative fluid velocity with respect to the shock front. These equations can be integrated immediately to obtain:

$$\begin{aligned} &\rho u = C_1; \\ &\rho u^2 + p - \sigma = C_2; \\ &\rho u^3 + 5pu - 2\sigma u + 2q = C_3, \end{aligned} \tag{45}$$

and integration constants can be obtained from boundary conditions at infinity, $\lim_{\xi\to\infty} \mathbf{v}(\xi) = (\rho_0, u_0, T_0)^T$ and $\lim_{\xi\to-\infty} \mathbf{v}(\xi) = (\rho_1, u_1, T_1)^T$:

$$C_1 = \rho_0 u_0 = \rho_1 u_1; \qquad C_2 = \rho_0 u_0^2 + p_0 = \rho_1 u_1^2 + p_1;$$
$$C_3 = \rho_0 u_0^3 + 5p_0 u_0 = \rho_1 u_1^3 + 5p_1 u_1.$$

Observe that σ and q vanish at infinity since equilibrium states are reached there. Introducing the following set of dimensionless variables:

$$\begin{aligned} &\hat{\rho} = \frac{\rho}{\rho_0}; \quad \hat{u} = \frac{u}{c_0}; \quad \hat{T} = \frac{T}{T_0}; \quad \hat{\sigma} = \frac{\sigma}{\rho_0 \frac{k}{m} T_0}; \quad \hat{q} = \frac{q}{\rho_0 \frac{k}{m} T_0 c_0}; \\ &\hat{\xi} = \frac{\rho_0 \alpha}{c_0 T_0^{r-1}} \xi; \quad M_0 = \frac{u_0}{c_0}; \quad c_0 = \sqrt{\frac{5}{3}\frac{k}{m} T_0}, \end{aligned} \tag{46}$$

where M_0 is Mach number and c_0 local speed of sound, equations (45) can be put into dimensionless form:

$$\begin{aligned}&\hat{\rho}\hat{u} = M_0;\\ &\frac{5}{3}\hat{\rho}\hat{u}^2 + \hat{\rho}\hat{T} - \hat{\sigma} = \frac{5}{3}M_0^2 + 1;\\ &\frac{5}{3}\hat{\rho}\hat{u}^3 + 5\hat{\rho}\hat{T}\hat{u} - 2\hat{\sigma}\hat{u} + 2\hat{q} = \frac{5}{3}M_0^3 + 5M_0\end{aligned} \tag{47}$$

whereas constitutive functions (42) combined with (43) become:

$$\hat{\sigma} = \frac{4}{3}\,\hat{T}^r\,\frac{d\hat{u}}{d\hat{\xi}}; \quad \hat{q} = -\frac{9}{4}\,\hat{T}^r\,\frac{d\hat{T}}{d\hat{\xi}}. \tag{48}$$

By putting $\hat{\sigma} = 0$, $\hat{q} = 0$ into (47) one can obtain the values of dimensionless variables behind the shock wave in terms of Mach number:

$$\hat{\rho}_1 = \frac{\rho_1}{\rho_0} = \frac{4M_0^2}{M_0^2 + 3} = \frac{u_0}{u_1} = \frac{1}{\hat{u}_1}; \quad \hat{T}_1 = \frac{T_1}{T_0} = \frac{5M_0^4 + 14M_0^2 - 3}{16M_0^2}. \tag{49}$$

Actually, solutions (49) are solutions of Rankine-Hugoniot equations for the system (40). Finally, combining (47) with (48) a system of two ordinary differential equations is obtained:

$$\begin{aligned}\frac{d\hat{u}}{d\hat{\xi}} &= F_u(\hat{u}, \hat{T}) = \frac{3}{4\,\hat{T}^r}\left\{M_0\left(\frac{5}{3}(\hat{u} - M_0) + \frac{\hat{T}}{\hat{u}}\right) - 1\right\};\\ \frac{d\hat{T}}{d\hat{\xi}} &= F_T(\hat{u}, \hat{T}) = -\frac{4}{9\,\hat{T}^r}\left\{\frac{M_0}{2}\left(\frac{5}{3}(\hat{u} - M_0)^2 - 3\hat{T} + 5\right) - \hat{u}\right\},\end{aligned} \tag{50}$$

which represent the system of shock structure equations supposed to be solved together with boundary conditions:

$$\lim_{\hat{\xi}\to\pm\infty} \frac{d\hat{\mathbf{v}}}{d\hat{\xi}}(\hat{\xi}) = \mathbf{0}; \quad \hat{\mathbf{v}}(\hat{\xi}) = (\hat{u}(\hat{\xi}), \hat{T}(\hat{\xi}))^T. \tag{51}$$

Shock waves are physically admissible for $M_0 > 1$ and our goal will be to determine the heteroclinic orbit connecting stationary points $(\hat{u}_0, \hat{T}_0) = (M_0, 1)$ for $\hat{\xi} \to \infty$ and $(\hat{u}_1, \hat{T}_1)$ for $\hat{\xi} \to -\infty$. In [7] it was done numerically because there is no analytical solution under assumption (43). Here approximate analytical solutions will be analyzed by means of general procedure outlined in Section 3.

5.2 Variational approximation

Variational principle (9) applied to the shock structure problem (50)-(51) reads:

$$J(\hat{\mathbf{V}}) = \int_{-\infty}^{\infty} \left\{ \left(\frac{d\hat{U}}{d\hat{\xi}} - F_u(\hat{U}, \hat{\theta}) \right)^2 + \left(\frac{d\hat{\theta}}{d\hat{\xi}} - F_T(\hat{U}, \hat{\theta}) \right)^2 \right\} d\hat{\xi} \to \min . \tag{52}$$

Approximate solution will be searched for in the following subset of admissible functions:

$$\begin{aligned} \tilde{D} = \Bigg\{ & \hat{\mathbf{V}}(\hat{\xi}) : \hat{\mathbf{V}}(\hat{\xi}) \in C^1(\mathbb{R}, \mathbb{R}^2); \lim_{\hat{\xi} \to -\hat{a}^+} \frac{d\hat{\mathbf{V}}}{d\hat{\xi}}(\hat{\xi}) = \\ & \lim_{\hat{\xi} \to \hat{a}^-} \frac{d\hat{\mathbf{V}}}{d\hat{\xi}}(\hat{\xi}) = 0; \frac{d\hat{\mathbf{V}}}{d\hat{\xi}}(\hat{\xi}) \equiv 0, \hat{\xi} \in \mathbb{R} \setminus (-\hat{a}, \hat{a}) \Bigg\} . \end{aligned} \tag{53}$$

Trial functions will be supposed in the form:

$$\hat{\mathbf{v}}^{(n)}(\hat{\xi}) = \begin{cases} \hat{\mathbf{v}}_1 = (\hat{u}_1, \hat{T}_1), & \hat{\xi} \in (-\infty, -\hat{a}], \\ (\hat{u}^{(n)}(\hat{\xi}), \hat{T}^{(n)}(\hat{\xi})), & \hat{\xi} \in (-\hat{a}, \hat{a}), \\ \hat{\mathbf{v}}_0 = (\hat{u}_0, \hat{T}_0), & \hat{\xi} \in [\hat{a}, \infty), \end{cases} \tag{54}$$

where $\hat{u}^{(n)}(\hat{\xi})$ and $\hat{T}^{(n)}(\hat{\xi})$ stand for n^{th}-degree polynomial approximation of the viscous profile.

In contrast to the solution (27) of Burgers' equation, solution of gas dynamics equations (50) do not possess symmetry properties. Consequently, a full polynomial approximation has to be used in the search for approximate solution. Another important remark is concerned with the fact that solution of (50)-(51) strongly depends on the value of Mach number M_0. Therefore, exact form of each particular approximation (54), i.e. coefficients of the polynomial, will also depend on M_0. In the sequel all the calculations will be performed for $M_0 = 2.5$ and $r = 0.64$ - experimentally determined value of r for monatomic gases like Ar. Corresponding stationary points are $(\hat{u}_0, \hat{T}_0) = (2.5, 1.0)$, $(\hat{u}_1, \hat{T}_1) = (0.925, 2.798)$.

As a first approximation a third degree polynomial will be used. In order to obtain $\hat{\mathbf{v}}^{(3)}(\hat{\xi}) \in \tilde{D}$ one must use the following profiles:

$$\begin{aligned} \hat{u}^{(3)}(\hat{\xi}) &= \frac{\hat{u}_0 + \hat{u}_1}{2} + \frac{3(\hat{u}_0 - \hat{u}_1)}{4\,\hat{a}}\,\hat{\xi} - \frac{\hat{u}_0 - \hat{u}_1}{4\,\hat{a}^3}\,\hat{\xi}^3; \\ \hat{T}^{(3)}(\hat{\xi}) &= \frac{\hat{T}_0 + \hat{T}_1}{2} + \frac{3(\hat{T}_0 - \hat{T}_1)}{4\,\hat{a}}\,\hat{\xi} - \frac{\hat{T}_0 - \hat{T}_1}{4\,\hat{a}^3}\,\hat{\xi}^3. \end{aligned} \tag{55}$$

Obviously, profiles have the same general form - only $\hat{u}$'s are replaced by $\hat{T}$'s. In such a way functional (52) becomes $J(\hat{\mathbf{v}}^{(3)}) = J(\hat{a})$ and from $dJ/d\hat{a} = 0$ one obtains:

$$\hat{a} = 2.410; \quad J^{(3)} = 5.423. \tag{56}$$

Although a fairly good approximation is obtained, the results could be improved by the use of higher order approximations. For example, using:

$$\begin{aligned} \hat{u}^{(4)}(\hat{\xi}) &= \frac{\hat{u}_0 + \hat{u}_1 + 2\,\hat{a}^4 a_4}{2} + \frac{3(\hat{u}_0 - \hat{u}_1)}{4\,\hat{a}}\,\hat{\xi} \\ &\quad - 2\,\hat{a}^2 a_4 \hat{\xi}^2 - \frac{\hat{u}_0 - \hat{u}_1}{4\,\hat{a}^3}\,\hat{\xi}^3 + a_4 \hat{\xi}^4, \end{aligned} \tag{57}$$

and $\hat{T}^{(4)}(\hat{\xi})$ obtained from $\hat{u}^{(4)}(\hat{\xi})$ by replacing $\hat{u}$'s with $\hat{T}$'s and a_4 with b_4, one obtains $J(\hat{\mathbf{v}}^{(4)}) = J(\hat{a}, a_4, b_4)$. Necessary conditions of extremum $\partial J/\partial \hat{a} = 0$, $\partial J/\partial a_4 = 0$ and $\partial J/\partial b_4 = 0$ yield:

$$\begin{gathered} \hat{a} = 2.925; \\ a_4 = 5.014 \times 10^{-3}; \quad b_4 = -4.245 \times 10^{-3}; \\ J^{(4)} = 5.349. \end{gathered} \tag{58}$$

For the final test a fifth degree approximation will be used:

$$\begin{aligned} \hat{u}^{(5)}(\hat{\xi}) = & \frac{\hat{u}_0 + \hat{u}_1 + 2\,\hat{a}^4 a_4}{2} + \frac{3(\hat{u}_0 - \hat{u}_1) + 4\,\hat{a}^5 a_5}{4\,\hat{a}}\,\hat{\xi} \\ & - 2\,\hat{a}^2 a_4 \hat{\xi}^2 - \frac{\hat{u}_0 - \hat{u}_1 + 8\,\hat{a}^5 a_5}{4\,\hat{a}^3}\,\hat{\xi}^3 + a_4 \hat{\xi}^4 + a_5 \hat{\xi}^5, \end{aligned} \tag{59}$$

with $\hat{T}^{(5)}(\hat{\xi})$ obtained in a similar way as before and with a_5 replaced with b_5. Thus, one obtains $J(\hat{\mathbf{v}}^{(5)}) = J(\hat{a}, a_4, b_4, a_5, b_5)$ and necessary conditions of extremum yield:

$$\begin{gathered} \hat{a} = 2.973; \\ a_4 = -7.096 \times 10^{-4}; \quad b_4 = 1.357 \times 10^{-3}; \\ a_5 = 1.964 \times 10^{-3}; \quad b_5 = -6.194 \times 10^{-4}; \\ J^{(5)} = 5.298. \end{gathered} \tag{60}$$

One may observe that the value of the functional (52) decreases with the increase of the order of approximation.

In Figure 2. graphs of numerical and approximate solutions are presented. They are shifted so that abscissas of the maximum slope points coincide. It can be observed that shapes of the profiles obtained by direct method resemble numerically obtained profile.

Furthermore, shock thickness defined as $\hat{\delta} = |(\hat{u}_1 - \hat{u}_0)/\max(d\hat{u}/d\hat{\xi})|$ could be used as another criterion of accuracy. Shock thicknesses evaluated at approximate solutions are:

$$\hat{\delta}^{(3)} = 3.214; \quad \hat{\delta}^{(4)} = 3.095; \quad \hat{\delta}^{(5)} = 2.854. \tag{61}$$

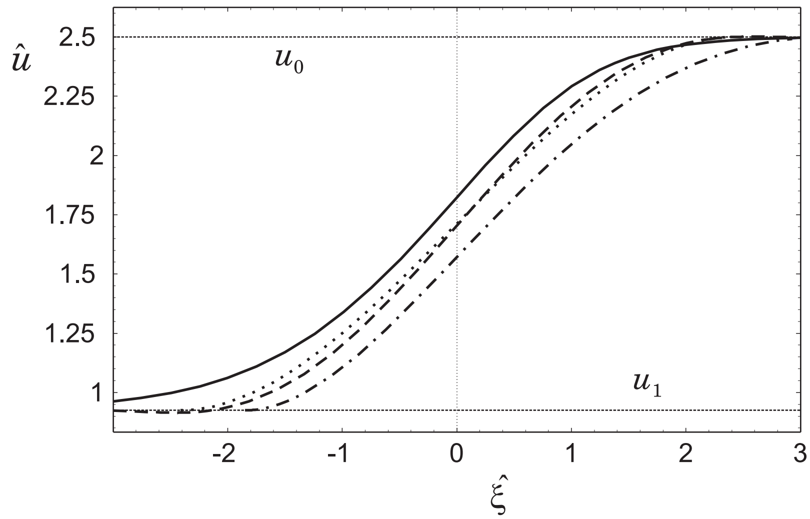

Figure 2: Numerical and approximate solutions for velocity profile of shock structure equations (50): $\hat{u}_{\mathrm{num}}(\hat{\xi})$ - solid, $\hat{u}^{(3)}(\hat{\xi})$ - dotted, $\hat{u}^{(4)}(\hat{\xi})$ - dash-dot, $\hat{u}^{(5)}(\hat{\xi})$ - dashed

At the same time shock thickness obtained by numerical integration of (50)-(51) reads $\hat{\delta}^{(E)} = 2.894$ which confirms that $\hat{\delta}^{(5)}$ gives the best approximation.

6 Conclusions

In this paper a variational approach is proposed to the problem of shock structure. Boundary-value problem (5),(7), which determines smooth profile of the shock wave with structure, consists of n first-order ordinary differential equations with $2n$ boundary conditions at $\pm\infty$. Since the order n of the system could be arbitrary, there does not exist variational formulation in the usual sense. Here, it was shown that shock structure problem can be related to a proper variational principle by means of least-squares method. Namely, variational problem (9) formulated on the set D of admissible functions (Eq. (10)) recovers governing equations (5) as necessary conditions of extremum, as well as boundary conditions (8) as consequences of transversality conditions. In the sequel this variational formulation is exploited in the search for approximate analytical solutions by means of Ritz direct method. For that purpose a subset $\tilde{D} \subset D$ (Eq. (14)) of admissible functions is used. This procedure is then applied in the analysis of shock structure in Burgers' equation and gas dynamics equations with viscosity and heat conduction. A good agreement of approximate and exact solutions is obtained, and convergence of approximations is observed. Moreover, good estimates of the shock thickness were also obtained.

Existence of variational formulation for the shock structure problem could be a good starting point for future studies. Namely, variational principle (9) is formulated without any reference to the mechanism of dissipation. Since relaxation profiles of the system (4) are governed by the ODE system of the same formal structure, this procedure can be applied to this class of problems as well. Also, it will be interesting to analyze the shock thickness in gas dynamics for a broad range of Mach numbers.

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Varijacioni pristup problemu strukture udarnog talasa

UDK 534.13, 534.21, 517.95

U ovom radu je izložen varijacioni pristup problemu strukture udarnog talasa. Za ovaj problem, koji je opisan sistemom od n običnih diferencijalnih jednačina prvog reda sa $2n$ graničnih uslova u $\pm\infty$, data je varijaciona formulacija u duhu metoda najmanjih kvadrata. Dobijeni varijacioni princip je prilagodjen primeni Ricovog metoda. Ovaj direktni metod je iskorišćen za konstrukciju približnih rešenja problema u analitičkoj formi i dobijanje ocene širine udarnog talasa. Predloženi postupak je primenjen u analizi Burgersove jednačine i jednačina gasne dinamike.