

A METHOD FOR SHOCK CALCULATION

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The mass, momentum and energy conservation laws allow shock and rarefaction waves to be present in the solution of continuum mechanics problems. When these problems are solved with homogeneous difference techniques, the strong shock surface is represented by a layer of a finite width within which the quantities vary continuously from a state before the shock front to a state behind it. These states are related by the strong shock conditions. Since they lie on the Hugoniot, there must exist a mechanism which maintains energy dissipation in the shock layer. One of these mechanisms is a method by Kuropatenko which uses the difference equations applicable for strong shocks. The method can be implemented in different difference schemes. The paper presents one of them, describes its basic properties, and provides results of some calculations.

Keywords: conservation laws, energy dissipation, difference scheme, shock, rarefaction.

Introduction

In 1D, the laws of mass, momentum and energy conservation for ideal continuum with no heat conduction in Lagrangian coordinates for the case of plane symmetry read as

$$\frac{\partial V}{\partial t} - \frac{\partial U}{\partial M} = 0, \quad (1)$$

$$\frac{\partial U}{\partial t} + \frac{\partial P}{\partial M} = 0, \quad (2)$$

$$\frac{\partial \varepsilon}{\partial t} + \frac{\partial (PU)}{\partial M} = 0, \quad (3)$$

where t is time, M is mass coordinate, U is material velocity, V is specific volume, P is pressure, $\varepsilon = E + 0.5U^2$ is specific total energy, and E is specific internal energy.

The system of equations (1)–(3) is closed by the equation of state

$$P = F(V, E) \quad (4)$$

and the equation of trajectory for a particle with coordinate M

$$\left(\frac{\partial x}{\partial t} \right)_M - U = 0, \quad (5)$$

where x is the Eulerian coordinate of the particle.

Since equations (1)–(3) are not linear, they allow strong and weak discontinuities to be present in continuum mechanics problems. Material states before and behind the shock front are related by the system of non-linear algebraic equations (Hugoniot conditions)

$$P_1 - P_0 - W(U_1 - U_0) = 0, \quad (6)$$

$$U_1 - U_0 + W(V_1 - V_0) = 0, \quad (7)$$

$$(E_1 + 0.5U_1^2 - E_0 - 0.5U_0^2)W - (P_1U_1 - P_0U_0) = 0. \quad (8)$$

Here W is strong shock velocity, and the subscript 0 corresponds to the state before the front and the subscript 1 corresponds to the state behind the front. Entropy jumps on the strong shock surface. This is the key difference between the shock waves and the waves where the quantities vary continuously.

When homogeneous difference methods are used for hydrodynamics, the strong shock surface is represented by a layer of a finite width [1, 2]. The strong shock smears [3]. In the layer, the quantities continuously vary from a state before the shock front to a state behind it. Since entropy jumps across the shock, there arises the question about the mechanism of energy dissipation in the shock layer. In the literature we can find four basically different mechanisms of energy dissipation [4, 7]. Consider a difference scheme based on the method proposed in [7].

1. Basic equations

The difference equations are written for a staggered mesh (Fig. 1). Velocities and coordinates are updated on the boundaries of intervals and the thermodynamic quantities are updated in their centers.

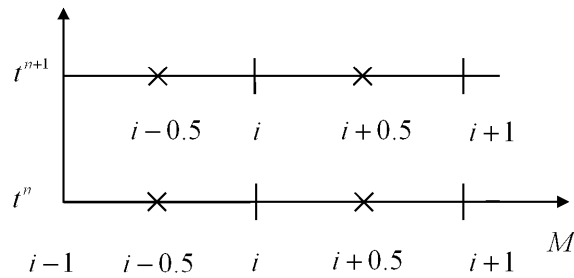


Fig. 1. Staggered mesh

All intervals are divided into those where material is compressed ($U_i^n - U_{i-1}^n < 0$) and those where material expands ($U_i^n - U_{i-1}^n \geq 0$). For the intervals of the first type, equations (1)–(5) are approximated by the difference equations

$$x_i^{n+1} = x_i^n + \tau U_i^n, \quad V_{i-0.5}^{n+1} = \frac{x_i^{n+1} - x_{i-1}^{n+1}}{\Delta M_{i-0.5}^n} \quad (9)$$

$$U_i^{n+1} = U_i^n - \frac{2\tau}{\Delta M_{i+0.5}^n + \Delta M_{i-0.5}^n} (\bar{P}_{i+0.5}^n - \bar{P}_{i-0.5}^n), \quad (10)$$

$$\varepsilon_{i-0.5}^{n+1} = E_{i-0.5}^n + 0.5(U_{i-0.5}^{*n})^2 - \frac{\tau}{\Delta M_{i-0.5}^n} (P_i^* U_i^n - P_{i-1}^* U_{i-1}^n), \quad (11)$$

$$P_{i-0.5}^{n+1} = F(V_{i-0.5}^{n+1}, E_{i-0.5}^{n+1}), \quad (12)$$

where $\Delta M_{i-0.5}^n = M_i^n - M_{i-1}^n$.

In equations (9)–(12) we use the auxiliary quantities \bar{P}^n , P^* and U^* . The quantity \bar{P}^n is derived from Hugoniot conditions (6)–(8) and ΔU^n which is known. The method to derive P^* and U^* will be described below.

For the intervals of the second type, the difference equations are written as

$$x_i^{n+1} = x_i^n + \tau U_i^n, V_{i-0.5}^{n+1} = \frac{x_i^{n+1} - x_{i-1}^{n+1}}{\Delta M_{i-0.5}^n} \quad (13)$$

$$U_i^{n+1} = U_i^n - \frac{2\tau}{\Delta M_{i+0.5}^n + \Delta M_{i-0.5}^n} (\bar{P}_{i+0.5}^n - \bar{P}_{i-0.5}^n), \quad (14)$$

$$E_{i-0.5}^{n+1} = E_{i-0.5}^n - \int_{V^n}^{V^{n+1}} P_{i-0.5}(V_{i-0.5}, E_{i-0.5}) dV, \quad (15)$$

$$P_{i-0.5}^{n+1} = F(V_{i-0.5}^{n+1}, E_{i-0.5}^{n+1}), \quad (16)$$

where $\bar{P}_{i-0.5}^n = P_{i-0.5}^n - a_{i-0.5}^n \kappa_{i-0.5} (U_i^n - U_{i-1}^n)$, $a_{i-0.5}^n = \rho_{i-0.5}^n c_{i-0.5}^n$, $c = \sqrt{\left(\frac{\partial P}{\partial \rho}\right)_s}$ is

adiabatic sound velocity, and $\kappa_{i-0.5} = \frac{\tau a_{i-0.5}^n}{\Delta M_{i-0.5}^n}$ is local Courant number. Internal energy at step $n+1$ is calculated by integrating (15) and (16) along the isentrope which ensures any predefined accuracy in the determination of entropy.

2. Determination of auxiliary quantities

The quantities P^* and U^* are defined on the following mesh (Fig. 2).

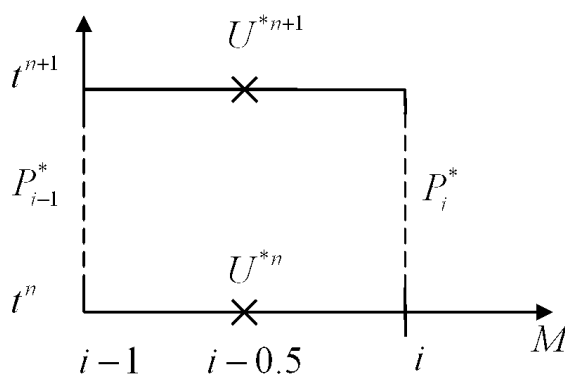


Fig. 2. Mesh for auxiliary functions

The values of P_i^* are defined by solutions in the intervals on the right and left from point i in accord with Table 1.

The quantity $U_{i-0.5}^{*n}$ for the intervals of the first type is defined with respect to the shock direction.

If $P_{i+0.5}^n < P_{i-1.5}^n$, the wave moves right $W_{i-0.5}^n > 0$ and $U_{i-0.5}^{*n} = U_i^n$.

If $P_{i+0.5}^n \geq P_{i-1.5}^n$, the wave moves left $W_{i-0.5}^n < 0$ and $U_{i-0.5}^{*n} = U_{i-1}^n$.

In the intervals of the second type $W_{i-0.5}^n = 0$ and $U_{i-0.5}^{*n}$ is calculated as the half-sum of boundary velocities: $U_{i-0.5}^{*n} = 0.5(U_{i-1}^n + U_i^n)$.

Table 1

The values of P_i^*

N	Interval $i - 0.5$ $\omega_L = W_{i-0.5}^n(U_i^n - U_{i-1}^n)$	Interval $i + 0.5$ $\omega_R = W_{i+0.5}^n(U_{i+1}^n - U_i^n)$	P_i^*
1	$\omega_L = 0$	$\omega_R = 0$	$P_i^* = 0.5(\overline{P}_{i-0.5}^n + \overline{P}_{i+0.5}^n)$
2	$\omega_L = 0$	$\omega_R < 0$	$P_i^* = 0.5(\overline{P}_{i-0.5}^n + P_{i+0.5}^n)$
3	$\omega_L = 0$	$\omega_R > 0$	$P_i^* = \overline{P}_{i+0.5}^n$
4	$\omega_L > 0$	$\omega_R = 0$	$P_i^* = 0.5(P_{i-0.5}^n + \overline{P}_{i+0.5}^n)$
5	$\omega_L > 0$	$\omega_R < 0$	$P_i^* = 0.5(P_{i-0.5}^n + P_{i+0.5}^n)$
6	$\omega_L > 0$	$\omega_R > 0$	$P_i^* = \overline{P}_{i+0.5}^n$
7	$\omega_L < 0$	$\omega_R = 0$	$P_i^* = \overline{P}_{i-0.5}^n$
8	$\omega_L < 0$	$\omega_R < 0$	$P_i^* = \overline{P}_{i-0.5}^n$
9	$\omega_L < 0$	$\omega_R > 0$	$P_i^* = 0.5(\overline{P}_{i-0.5}^n + \overline{P}_{i+0.5}^n)$

The quantity $U_{i-0.5}^{*n+1}$ which is needed for the determination of internal energy $E_{i-0.5}^{n+1} = \varepsilon_{i-0.5}^{n+1} - 0.5(U_{i-0.5}^{*n+1})^2$, is calculated from the equation

$$U_{i-0.5}^{*n+1} = U_{i-0.5}^{*n} - \frac{\tau}{\Delta M_{i-0.5}}(P_i^* - P_{i-1}^*).$$

3. Basic properties of the difference scheme

3.1. Approximation errors

According to [8], the differential conservation laws are written as

$$\begin{aligned} \frac{\partial x}{\partial t} - U &= \omega_4, \quad \frac{\partial x}{\partial M} - V = \omega_5, \\ \frac{\partial U}{\partial t} + \frac{\partial P}{\partial M} &= \omega_2, \\ \frac{\partial \varepsilon}{\partial t} + \frac{\partial(PU)}{\partial M} &= \omega_3, \end{aligned}$$

where the approximation errors ω_4 , ω_5 , ω_2 and ω_3 for an acoustically approximated shock ($W = a$) are as follows

$$\begin{aligned} \omega_4 &= -\frac{\tau}{2}\dot{U} + \frac{\tau^2}{12}\ddot{U} + o(\tau^3), \quad \omega_5 = -V''\frac{h^2}{24} + o(h^3), \\ \omega_2 &= -\frac{\tau}{2}\ddot{U} - \frac{\tau^2}{6}\dddot{U} + ahU'' - \frac{h^2}{24}P''' + o(\tau^3, h^3), \\ \omega_3 &= -\frac{\tau}{2}\ddot{\varepsilon} - \frac{\tau^2}{6}\dddot{\varepsilon} - h\left(\frac{1}{2}P'U' + \frac{1}{2}P''U - a(U')^2 - aUU''\right) + o(\tau^3, h^2). \end{aligned}$$

For the rarefaction wave, they are

$$\omega_4 = -\frac{\tau}{2}\dot{U} + \frac{\tau^2}{12}\ddot{U} + o(\tau^3), \omega_5 = -V''\frac{h^2}{24} + o(h^3),$$

$$\omega_2 = -\tau\left(\frac{\ddot{U}}{2} - a^2U''\right) - \frac{\tau^2}{6}\ddot{U} - \frac{h^2}{24}P''' + o(\tau^3, h^3).$$

The entropy production equation for rarefaction is $T \left(\frac{\partial S}{\partial t} \right)_M = 0$.

Thus the approximation errors are first order infinitesimals in τ and ΔM on the shock wave, and first order infinitesimal in time and second order infinitesimal in the Lagrangian coordinate on the rarefaction wave.

3.2. Stability condition

Theorem 1. *The difference scheme under consideration is conditionally stable.*

Proof.

We use harmonics. For finding the stability condition, we write the difference scheme in the acoustic case

$$\frac{U_i^{n+1} - U_i^n}{\tau} + \frac{\bar{P}_{i+0.5}^n - \bar{P}_{i-0.5}^n}{h} = 0; \frac{P_{i+0.5}^{n+1} - P_{i+0.5}^n}{\tau} + a^2 \frac{U_{i+1}^n - U_i^n}{h} = 0. \quad (17)$$

Substituting

$$\delta P_{i+0.5}^n = \delta P_0 e^{\alpha t^n + i\beta m_{i+0.5}}, \delta U_i^n = \delta U_0 e^{\alpha t^n + i\beta m_i}, e^{\alpha\tau} = \lambda, e^{i\beta \frac{h}{2}} = \xi$$

yields

$$U_0(\lambda - 1 - \frac{\tau a}{h}(\xi^2 - 2 + \xi^{-2})) + \frac{\tau}{h}P_0(\xi - \xi^{-1}) = 0,$$

$$\frac{\tau a^2}{h}U_0(\xi - \xi^{-1}) + P_0(\lambda - 1) = 0.$$

The determinant of this system is

$$(\lambda - 1)^2 - \varkappa(\lambda - 1)(\xi^2 - 2 + \xi^{-2}) - \varkappa^2(\xi^2 - 2 + \xi^{-2}) = 0,$$

where $\varkappa = \frac{\tau a}{h}$. We solve this equation and obtain that $|\lambda| \leq 1$ at $\frac{\tau a}{h} \leq 1$. □

3.3. Monotony condition

Let a shock move to the right from point i ($W > 0$). On the shock, equations (17) take the form

$$U_{i+0.5}^{n+1} = U_{i+0.5}^n - \frac{\tau}{\Delta M_{i+0.5}}(P_{i+1}^* - P_i^*), P_{i+0.5}^{n+1} = P_{i+0.5}^n - \frac{\tau a^2}{h}(U_{i+1}^n - U_i^n). \quad (18)$$

Velocity in interval $(i + 0.5)$ is constant and equal to U_{i+1}^n . All quantities in interval $(i + 0.5)$ are before the shock front. With $P_i^* = P_{i+0.5}^n - W_{i+0.5}^n(U_{i+1}^n - U_i^n)$ and $P_{i+1}^* = P_{i+1.5}^n - W_{i+1.5}^n(U_{i+2}^n - U_{i+1}^n)$ equation (18) takes the form

$$U_{i+0.5}^{n+1} = U_{i+0.5}^n - \frac{\tau}{h}((P_{i+1.5}^n - P_{i+0.5}^n) - a(U_{i+1.5}^n - 2U_{i+0.5}^n + U_{i-0.5}^n)), \quad (19)$$

$$P_{i+0.5}^{n+1} = P_{i+0.5}^n - \frac{\tau a^2}{h}(U_{i+0.5}^n - U_{i-0.5}^n). \quad (20)$$

With the Riemann invariants $\alpha = P + aU, \beta = P - aU$, we convert (19)–(20) to

$$\begin{aligned} \alpha_{i+0.5}^{n+1} - \beta_{i+0.5}^{n+1} &= \alpha_{i+0.5}^n - \beta_{i+0.5}^n - \varkappa(\alpha_{i+1.5}^n + \beta_{i+1.5}^n - \alpha_{i+0.5}^n - \beta_{i+0.5}^n) + \\ &+ \varkappa(\alpha_{i+1.5}^n - \beta_{i+1.5}^n - 2(\alpha_{i+0.5}^n - \beta_{i+0.5}^n) + \alpha_{i-0.5}^n - \beta_{i-0.5}^n), \end{aligned}$$

$$\alpha_{i+0.5}^{n+1} + \beta_{i+0.5}^{n+1} = \alpha_{i+0.5}^n + \beta_{i+0.5}^n - \varkappa(\alpha_{i+0.5}^n - \beta_{i+0.5}^n - \alpha_{i-0.5}^n + \beta_{i-0.5}^n).$$

Summing these equation gives

$$2\alpha_{i+0.5}^{n+1} = 2(1 - \varkappa)\alpha_{i+0.5}^n + 2\varkappa\alpha_{i-0.5}^n + 4\varkappa\beta_{i+0.5}^n - 2\varkappa\beta_{i+1.5}^n - 2\varkappa\beta_{i-0.5}^n.$$

Taking into account that for a right moving wave, $\beta = const$, we obtain

$$\alpha_{i+0.5}^{n+1} = (1 - \varkappa)\alpha_{i+0.5}^n + \varkappa\alpha_{i-0.5}^n. \quad (21)$$

By Godunov's theorem, a scheme is monotone if coefficients in (21) are non-negative. This is true at $\varkappa \leq 1$.

Do similar manipulations for rarefaction. In this case, equations (17) with $\overline{P}_{i-0.5}^n = P_{i-0.5}^n - a_{i-0.5}^n \varkappa(U_i^n - U_{i-1}^n)$ take the form

$$U_i^{n+1} = U_i^n - \frac{\tau}{h}(P_{i+0.5}^n - P_{i-0.5}^n) + \varkappa^2(U_{i+1}^n - 2U_i^n + U_{i-1}^n), \quad (22)$$

$$P_{i+0.5}^{n+1} = P_{i+0.5}^n - a\varkappa(U_{i+1}^n - U_i^n). \quad (23)$$

Substituting yields

$$\alpha_i^{n+1} - \beta_i^{n+1} = \alpha_i^n - \beta_i^n - \varkappa(\alpha_{i+0.5}^n + \beta_{i+0.5}^n - \alpha_{i-0.5}^n - \beta_{i-0.5}^n) + \varkappa^2(\alpha_{i+1}^n - \beta_{i+1}^n - 2(\alpha_i^n - \beta_i^n) + \alpha_{i-1}^n - \beta_{i-1}^n),$$

$$\alpha_{i+0.5}^{n+1} + \beta_{i+0.5}^{n+1} = \alpha_{i+0.5}^n + \beta_{i+0.5}^n - \varkappa(\alpha_{i+1}^n - \beta_{i+1}^n - \alpha_i^n + \beta_i^n).$$

Summing with account for $\beta = const$ gives

$$\alpha_i^{n+1} = 0.5\varkappa^2\alpha_{i+1}^n - \varkappa\alpha_{i+0.5}^n + (1 - \varkappa^2)\alpha_i^n + \varkappa\alpha_{i-0.5}^n + 0.5\varkappa^2\alpha_{i-1}^n.$$

One of the coefficients is negative and therefore the scheme is non-monotone on rarefaction waves.

4. Generalization to spherical and cylindrical cases

In 1D, hydrodynamic equations for ideal medium read as

$$\left(\frac{\partial r}{\partial t}\right)_M = U, V = \frac{\partial r^\alpha}{\partial M}, \quad (24)$$

$$\frac{\partial U}{\partial t} + \alpha r^{\alpha-1} \frac{\partial P}{\partial M} = 0, \quad (25)$$

$$\frac{\partial \varepsilon}{\partial t} + \frac{\partial(\alpha r^{\alpha-1} U P)}{\partial M} = 0, \quad (26)$$

where α is dimensionality ($\alpha = 1$ for plane, $\alpha = 2$ for cylinder, and $\alpha = 3$ for sphere), and the Lagrangian coordinate M reads as

$$M = \int_0^r \rho r^{\alpha-1} dr.$$

Equations (24)–(26) in finite differences are written as

$$r_i^{n+1} = r_i^n + \tau U_i^n, V_{i-0.5}^{n+1} = \frac{(r_i^{n+1})^\alpha - (r_{i-1}^{n+1})^\alpha}{\Delta M_{i-0.5}^n},$$

$$U_i^{n+1} = U_i^n - \alpha (r_i^n)^{\alpha-1} \frac{\tau}{M_{i+}^n + \Delta M_{i-}^n} (P_{i+0.5}^n - P_{i-0.5}^n),$$

$$\varepsilon_{i-0.5}^{n+1} = E_{i-0.5}^n + 0.5(U_{i-0.5}^{*n})^2 - \alpha \frac{\tau}{\Delta M_{i-0.5}^n} ((r_i^n)^{\alpha-1} P_i^* U_i^n - (r_{i-1}^n)^{\alpha-1} P_{i-1}^* U_{i-1}^n),$$

where $M_{i-}^n = \rho_{i-0.5}^n ((r_i^n)^\alpha - (r_{i-0.5}^n)^\alpha)$ is the mass of a half of interval i and $M_{i+}^n = \rho_{i+0.5}^n ((r_{i+0.5}^n)^\alpha - (r_i^n)^\alpha)$ is the mass of a half of interval $i+1$ (see Fig. 3). For plane with $\alpha = 1$, these masses equal the halves of the masses of the intervals.

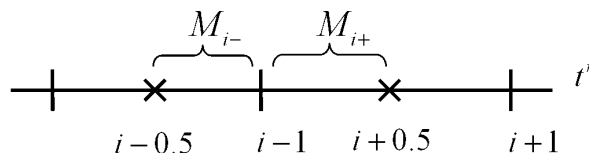


Fig. 3. Mesh

The auxiliary quantity $U_{i-0.5}^{*n+1}$ is calculated from the equation of motion

$$U_{i-0.5}^{*n+1} = U_{i-0.5}^{*n} - \alpha (r_{i-0.5}^n)^{\alpha-1} \frac{\tau}{\Delta M_{i-0.5}^n} (P_i^* - P_{i-1}^*).$$

5. Verification

The figures below compare results for some problems from [9] which were calculated with the proposed scheme, and their analytical solutions. All calculations were done with Courant number 0.5.

Example 1. Propagation of a stationary shock in ideal gas.

At the initial time $t = 0$, ideal gas, $\gamma = 4/3$, is in the region $0 \leq x \leq 14$.

Initial conditions: $\rho_0 = 1$, $E_0 = 0$, $P_0 = 0$, $U_0 = 0$.

Boundary conditions: $U_L = 3$, $U_R = 0$. A uniform mesh of 100 intervals was used.

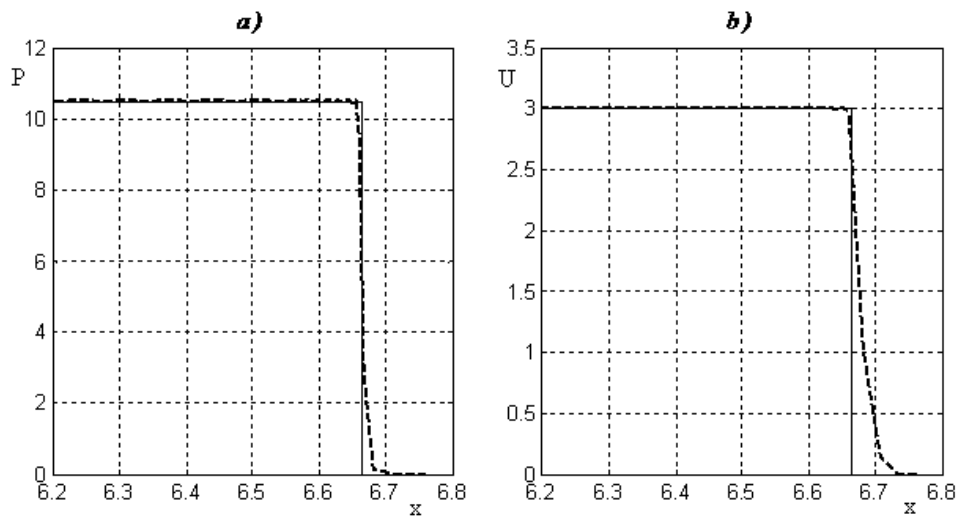


Fig. 4. Pressure and velocity in the stationary shock

Figures 4a and 4b show $P(x)$ and $U(x)$ profiles at $t = 1.904$. The solid line shows the analytical solution and the dashed one shows calculation with the proposed method.

Example 2. Propagation of a rarefaction wave in ideal gas.

At the initial time $t = 0$, ideal gas, $\gamma = 2$, is in the region $0 \leq x \leq 14$.

Initial conditions: $\rho_0 = 4.5$, $E_0 = 1.125$, $P_0 = 5.0625$, $U_0 = 0$.

Boundary conditions: $U_L = -1$, $U_R = 0$. A uniform mesh of 100 intervals was used.

Figures 5a and 5b show $P(x)$ and $U(x)$ profiles at $t = 4.043$. The solid line shows analytics

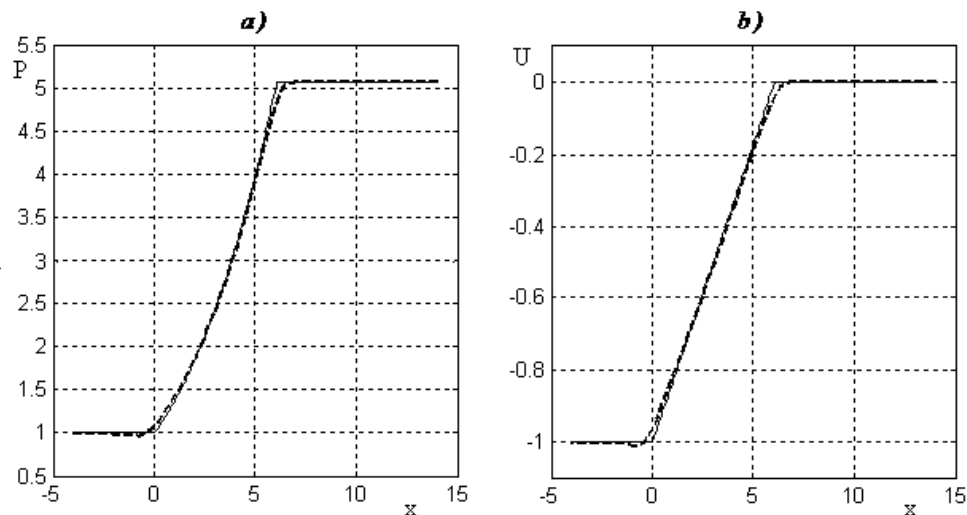


Fig. 5. Pressure and velocity in the rarefaction wave

and the dashed one shows calculation with the proposed method.

Example 3. A spherically symmetric shock converging to the center.

At the initial time $t = 0$, the cold ideal gas, $\gamma = 5/3$, is at rest in the region $0 \leq r \leq 1$. Initial conditions: $\rho_0 = 1$, $E_0 = 0$, $P_0 = 0$, $U_0 = 0$.

The condition on the boundary of the gas sphere is taken from the analytical solution [9] as a table of U versus t (Table 2).

Table 2

N	t	U_R	N	t	U_R
1	0	-1	9	0.328273	-1.04392
2	0.02	-1.004474	10	0.36	-1.0395
3	0.102828	-1.02181	11	0.39144	-1.03309
4	0.16	-1.0323	12	0.42	-1.0227
5	0.20701	-1.0391	13	0.438247	-1.01479
6	0.241516	-1.04277	14	0.475136	-0.991499
7	0.286642	-1.04513	15	0.50547	-0.964469
8	0.31	-1.045	16	0.540474	-0.92164

A uniform mesh of 200 intervals was used.

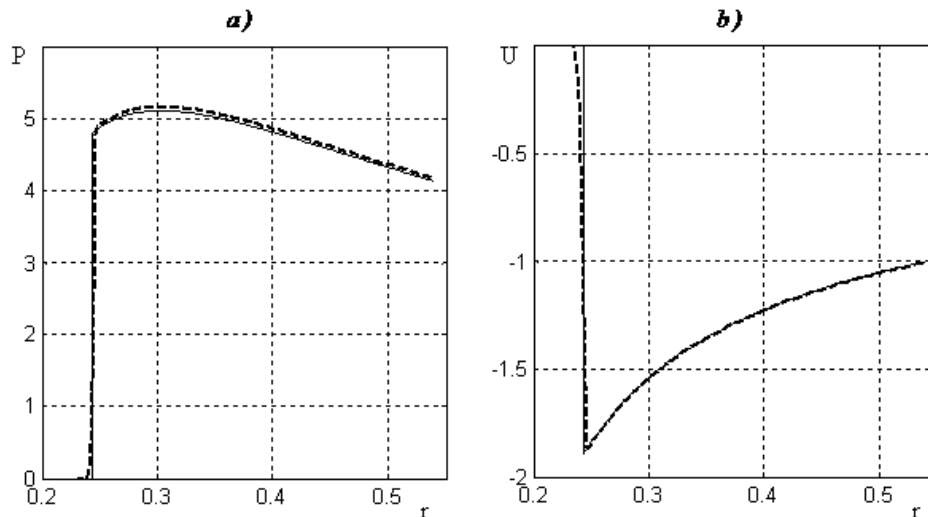


Fig. 6. Pressure and velocity in the spherically symmetric shock

Figures 6a and 6b show $P(r)$ and $U(r)$ profiles at $t = 0.45$. The solid line shows analytics from [9] and the dashed one shows calculation with the proposed method.

Example 4. Shock interaction with interface at $\frac{\rho_R}{\rho_L} = 0.5$ in ideal gas.

At the initial time $t = 0$, gas with the initial state $\rho_0 = 1$, $E_0 = 0$, $P_0 = 0$, $U_0 = 0$ is in the region $0 \leq r \leq 14$, and gas with the initial state $\rho_0 = 0.5$, $E_0 = 0$, $P_0 = 0$, $U_0 = 0$ is in the region $14 \leq r \leq 28$. In both the regions, the equation of state is ideal gas with $\gamma = 4/3$.

Boundary conditions: $U_L = 3$, $U_R = 0$.

A uniform mesh was used with 200 intervals in the first region and 100 intervals in the second one.

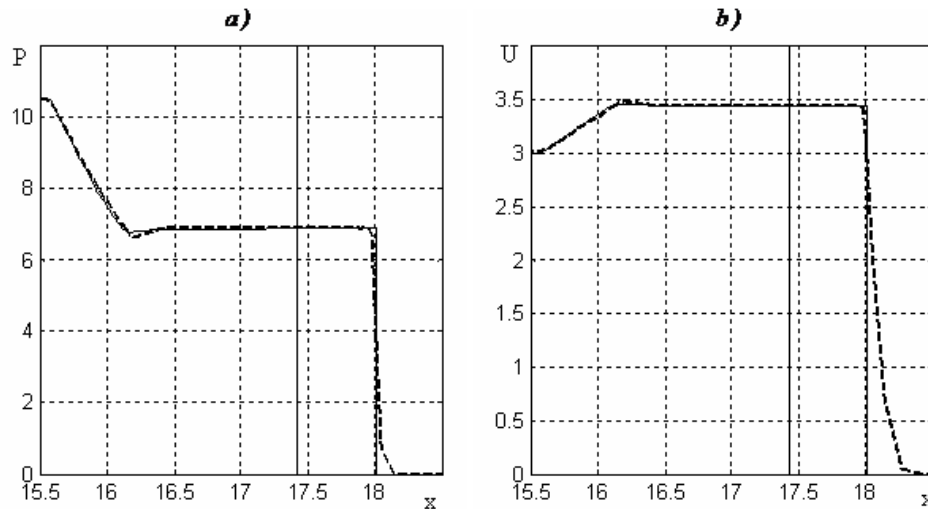


Fig. 7. Pressure and velocity in the shock interaction

Figures 7a and 7b show $P(x)$ and $U(x)$ profiles at $t = 5$. The solid line shows calculation by the VOLNA code [9] with shock capturing, and the dashed one shows calculation with the proposed method. The vertical line at $x = 17.44$ shows the position of the interface at that time.

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