# ANALYSIS OF SOME MODIFICATIONS OF THE LARGE-PARTICLE METHOD TO MODEL WAVE DYNAMICS PROBLEMS

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We perform a numerical analysis of various modifications of the large-particle method applied to problems of wave dynamics (gas dynamics). We use modifications of the large-particle method to solve the problems on calculation of the decay of an arbitrary discontinuity, propagation of shock waves and propagation of rarefaction waves. Calculations of the propagation of stationary shock waves show that all considered modifications of the large-particle method allow to calculate correctly a pressure behind the shock wave, despite the fact that a width of the shock transition zone and a profile of the shock wave pressure in the zone depend on the modification of the large-particle method. During solving the problem on the decay of an arbitrary discontinuity, we show that the solution obtained by modified large-particle method with recalculation of pressure at the Euler stage best coincides with the analytical solution to the problem, both in the region of the shock wave and in the rarefaction wave region. A significant advantage of this modification is the fact that the considered problems can be solved without introducing the "artificial" viscosity into the laws of conservation.

Keywords: shock wave; decay of an arbitrary discontinuity; Courant number; artificial viscosity; large particles.

## Introduction

Nowadays, mathematical modeling is a full-fledged tool for research on a wide range of problems of gas dynamics due to the active development of computer technology. Usually, in the case of fast process, mathematical modeling is the only way to obtain reliable information about the gas streams under study. In order to carry out numerical experiments, it is necessary to develop and adapt a computational tool, which allows to solve a wide range of practical problems.

At the present time, there is a sufficiently large number of numerical methods to solve the problems of continuum mechanics. Nevertheless, the large-particle method (LPM) proposed by O. M. Belotserkovskii and Yu. M. Davydov [1] is quite actively developed and used to solve a wide range of problems of gas dynamics. This method develops the method of particles in cells proposed by F. Harlow [2]. The method is based on the consistent use of the Euler and Lagrange approaches with the help of approximations in the fixed nodes of the computational grid and the subsequent consideration of an interaction of the calculated cells as independent large particles of liquid. There are the following two reasons of the interest in LPM. First, obvious advantages of these schemes are simplicity and physicality, as well as monotonicity, which ensures a good through account of discontinuous solutions. Second, there is a real possibility to obtain sufficiently exact solutions with the help of modern computer technology. The special advantage of LPM is a high scheme approximation viscosity based on the "divergent" differential equations of conservation. Advantages of the equations are most noticeable during calculations in Euler coordinates. The method allows to split by physical processes in order to solve problems with phase and chemical transformations.

The practical application of mathematical models more often sets the problems on detailed calculation of nonstationary gas-dynamic streams of multiphase disperse medium. Here the medium is a heterogeneous mixture of gaseous phase carrier and small suspended inclusions ("particles"), which are in a solid or liquid state. The possibilities of an analytic study of the nonstationary streams of such interpenetrating dissipative mediums are strongly limited. However, the majority of actual problems can be solved numerically with sufficient accuracy [3–7]. In order to describe the motion of a multiphase medium, it is necessary to use a much larger number of basic differential equations in comparison with a conventional single-phase medium. Therefore, the questions on speed of the algorithms become important in the calculation of time for transitions from one layer to another. To this end, in order to numerically integrate nonstationary equations of multiphase motion, explicit methods of payable through account having first-order of accuracy are used. The methods are logically simple and have the minimum possible volume of calculation formulas. Therefore, new modifications of LPM [8, 9] appear.

The purpose of this research is to analyze capabilities of LPM modifications given in [8, 9] in solving problems, which are of interest for the study of the following fast process:

1) calculation of the decay of an arbitrary discontinuity;

2) propagation of shock waves;

3) propagation of rarefaction waves.

# 1. Problem Statement and Description of Modifications of the Large-particle Method

### 1.1. Problem Statement

Consider one-dimensional motion of an ideal compressible gas described by differential Euler equations in a divergent form (equations of continuity, momentum, and energy)

$$\frac{\partial \rho}{\partial t} + div(\rho u) = 0, 
\frac{\partial \rho u}{\partial t} + div(\rho u u) + \frac{\partial p}{\partial x} = 0, 
\frac{\partial \rho E}{\partial t} + div(\rho E u) + div(p u) = 0.$$
(1)

The system (1) is supplemented with the equation of state

$$p = e\rho(\gamma - 1),$$

as well as with the equation of the specific total energy of the gas

$$E = e + \frac{u^2}{2}.$$

Here p,  $\rho$ , u, E, e, t, x,  $\gamma$  are pressure, density, velocity, specific total and internal energies, time, Cartesian coordinate and Poisson adiabatic exponent, respectively. In accordance with the considered problems, the system of conservation laws is supplemented with initial and boundary conditions.

#### 1.2. Description of the Large-particle Method

An idea of the method is to split by physical processes the initial non-stationary system of Euler equations (1), where the conservation laws are written in divergent form. Here the medium is modeled by a system of liquid (large) particles that coincide with cells of the Euler grid at the given time. The calculation of each time step is divided into the following three stages [1].

*I. Euler stage.* Neglect all effects associated with motion of a unit cell (there is no mass stream through the cell boundaries), and take into account effects of liquid acceleration obtained only due to pressure. Determine intermediate values of the unknown stream parameters for a large particle.

*II. Lagrange stage.* Calculate mass streams through boundaries of Euler cells when the liquid moves.

*III. Final stage.* Determine final values of the gas dynamic parameters of the stream at a new time point. To this end, use the laws of conservation of mass, momentum and energy for each cell and whole system on a fixed calculation grid.

Let us consider Euler stage of the calculation cycle for the one-dimensional plane case. If the density field is stagnated and the effects of medium displacement are not taken into account, then the preliminary values of velocity and total energy are determined by the following formulas:

$$\tilde{u}_{i}^{n} = u_{i}^{n} - \frac{p_{i+1/2}^{n} - p_{i-1/2}^{n}}{\Delta x} \frac{\Delta t}{\rho_{i}^{n}},$$
(2)

$$\tilde{E}_{i}^{n} = E_{i}^{n} - \frac{p_{i+1/2}^{n} u_{i+1/2}^{n} - p_{i-1/2}^{n} u_{i-1/2}^{n}}{\Delta x} \frac{\Delta t}{\rho_{i}^{n}},$$
(3)

where  $p, \rho, u, E, t, x$  are pressure, density, velocity, total energy, time, and Cartesian coordinates, respectively. Values with fractional indices relating to cell boundaries are as follows:

$$u_{i+1/2}^n = \frac{u_i^n + u_{i+1}^n}{2}, \ p_{i+1/2}^n = \frac{p_i^n + p_{i+1}^n}{2}.$$

We can use p + q instead of p in the formulas (2) and (3). Here q is a pseudo-viscosity. In this paper, we use a linear combination of quadratic and linear pseudo-viscosity, which is determined on the cell boundaries:

$$q_{i+1/2} = \begin{cases} A_q \rho_{i+1/2} c_{i+1/2} \Delta u_{i+1/2} + B_q \rho_{i+1/2} (\Delta u)_{i+1/2}^2, & \text{if } \Delta u_{i+1/2} > 0, \\ 0, & \text{if } \Delta u_{i+1/2} < 0, \end{cases}$$

$$q_{i-1/2} = \begin{cases} -A_q \rho_{i-1/2} c_{i-1/2} \Delta u_{i-1/2} - B_q \rho_{i-1/2} (\Delta u)_{i-1/2}^2, & \text{if } \Delta u_{i-1/2} < 0, \\ 0, & \text{if } \Delta u_{i-1/2} < 0, \end{cases}$$

$$\Delta u_{i+1/2} = u_i^n - u_{i+1}^n,$$

$$\Delta u_{i-1/2} = u_i^n - u_{i-1}^n, \end{cases}$$

$$(4)$$

where  $A_q$  and  $B_q$  are the coefficients of linear and quadratic pseudo-viscosity.

Then Lagrange and final stages follow. This completes the calculation cycle of the method.

#### 1.3. Some Modifications of the Large-particle Method

First, we consider the modification of LPM proposed by Grishin Yu. A. and Zenkin V. A. [9] in order to increase stability of the computational algorithm of LPM. In this modification, other formulas are proposed to calculate preliminary pressure, velocity, and total energy at the Euler stage.

The preliminary pressure for i - 1/2 and i + 1/2 boundaries between the cells i - 1, i and i + 1 on the n + 1 time layer are determined by the formula

$$\tilde{p}_{i+1/2}^{n+1} = \frac{p_{i+1}^n - p_i^n}{2} \left( 1 - (\gamma - 1)(u_{i+1}^n - u_i^n) \frac{\Delta t}{\Delta x} \right),\tag{5}$$

where  $\gamma$  is the Poisson adiabatic exponent.

Then obtained values are used in the formula (2) in order to determine the preliminary velocities in the cells. The formula (3) is replaced with the following:

$$\tilde{E}_{i}^{n+1} = E_{i}^{n} - \frac{\tilde{p}_{i+1/2}^{n}\tilde{u}_{i+1/2}^{n} - \tilde{p}_{i-1/2}^{n}\tilde{u}_{i-1/2}^{n}}{\Delta x} \frac{\Delta t}{\rho_{i}^{n}}.$$
(6)

Lagrange and final stages are carried out similarly to the basic LPM.

Another modification proposed by Grishin Yu.A. and Bakulin V.N. [9] is an implicit LPM scheme that does not require iterations at the calculation step. In order to carry out the calculation, the numbers of cells are consecutively considered in increasing order. Therefore, the intermediate parameters for i - 1 cells in (n + 1)-th time point are already known. The intermediate pressure in the cell at the Euler stage is determined as follows:

$$\tilde{p}_{i}^{n+1} = \frac{\left\{ p_{i}^{n} - (\gamma - 1) \frac{\Delta t}{\Delta x} p_{i}^{n+\frac{1}{2}} \left\{ \frac{1}{2} \left\{ u_{i}^{n} + u_{i+1}^{n} - \left[ \frac{p_{i+1}^{n}}{2} - p_{i-\frac{1}{2}}^{n+\frac{1}{2}} \right] \frac{\Delta t}{\Delta x \rho_{i}^{n}} \right\} - u_{i-\frac{1}{2}}^{n+\frac{1}{2}} \right\} \right\}}{\left[ 1 - \frac{1}{4\rho_{i}^{n}} \left(\gamma - 1\right) p_{i}^{n+\frac{1}{2}} \left( \frac{\Delta t}{\Delta x} \right)^{2} \right]}, \quad (7)$$

where

$$p_i^{n+\frac{1}{2}} = \frac{\tilde{p}_{i-1}^{n+1} + p_{i+1}^n}{2},$$
$$X_{i-\frac{1}{2}}^{n+\frac{1}{2}} = \frac{\tilde{X}_{i-1}^{n+1} + X_i^n}{2}, \quad X = (p, u).$$

After calculation of the intermediate pressures, the preliminary values of velocity in the cells are determined:

$$\tilde{u}_{i}^{n+1} = u_{i}^{n} - \left(\frac{\tilde{p}_{i}^{n+1} + p_{i+1}^{n}}{2} - p_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right) \frac{\Delta t}{\Delta x \rho_{i}^{n}}.$$
(8)

The Euler stage is completed by calculation of the total energy and correction of the density by the formulas:

$$\tilde{E}_{i}^{n+1} = \frac{\tilde{p}_{i}^{n+1}}{(\gamma - 1)\rho_{i}^{n}} + \frac{\left(\tilde{u}_{i}^{n+1}\right)^{2}}{2},\tag{9}$$

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$$\rho_i^{n+1} = \rho_i^n \left( 1 + \frac{u_{i+1} - u_{i-1}}{2\Delta x} \Delta t \right)^{-1}.$$
 (10)

Then the Lagrange and final stages of LPM follow. Note that the second modification corresponds to the concept of an implicit scheme, since there are parameters of *n*-th and (n + 1)-th time points in the formulas (7) - (9). At the Euler stage of the basic LPM, the cell density is set to be  $\rho = const$ . The method described above can be used both in combination with the basic LPM, and with the modification.

### 2. Numerical Experiment

#### 2.1. Propagation of a Stationary Shock Wave

Let us consider the propagation of a stationary shock wave (SW) for the following relation between a dimensionless pressure on a shock change and the pressure of an unperturbed medium:  $P/P_0 = 5$ , 10. The remaining parameters of the medium in the unperturbed stream region at the initial time point t = 0 are the following:  $\rho = 1$ , U = 0, E = 0,  $P_0 = 1$ , and on the boundary the parameters are determined by the Rankine – Hugoniot condition.

The graphs of pressure of stationary shock waves are given in Fig. 1 and 2. The graphs are obtained by the basic LPM, the modification [8], the modification [9] such that the specific total energy at the Euler stage is calculated by the formulas (6) and (9). Also, the graphs of the analytical solution for the dimensionless pressures  $P/P_0 = 5$ , 10 are given in Fig. 1 and 2. All calculations were carried out for the Courant net number Co = 0.3by the basic LPM and the modifications of LPM described in the papers [8] and [9]. All these methods calculate the pressure and velocity profiles very well. However, during the calculation of the modified LPM [9], it turned out that the specific total energy at the shock change is overestimated in comparison with the analytical solution of the considered problem. In order to solve the problem, we replace the equation (9) with the equation (6) at the Euler stage.

In Fig. 1 and 2, dot-dash line represents the basic LPM, dots with circles are the modified LPM [8], dots with asterisks are the modified LPM [9] such that the total energy is calculated by the formula (9), solid line is the modified LPM [9] such that the total energy is calculated by the formula (6), dashed line is the analytical solution.

Calculations of the propagation of stationary SW given in Fig. 1 and 2 show that all modifications of LPM allow to calculate correctly a pressure behind SW, despite the fact that a width of the shock transition zone and a profile of the SW pressure in the zone depend on the modified LPM.

### 2.2. Decay of an Arbitrary Discontinuity

Consider the problem on the decay of an arbitrary discontinuity. An infinite pipe is filled with air ( $\gamma = 1.4$ ) and divided by a partition at the point x = 0. For t = 0, the gas state is described by the following function:

$$\begin{pmatrix} \rho \\ u \\ p \end{pmatrix} \bigg|_{t=0} = \begin{cases} (\rho_L \ 0 \ p_L), & x \le 0, \\ (\rho_R \ 0 \ p_R), & x > 0. \end{cases}$$



Fig. 1. Profiles of stationary SW for various modifications of LPM at time  $t = 0.3236, P/P_0 = 5$ 



Fig. 2. Profiles of stationary SW for various modifications of LPM at time  $t = 0.2019, P/P_0 = 10$ 

Here  $\rho_L$ ,  $p_L$ ,  $\rho_R$ ,  $p_R$  are the density and pressure in front of the partition and behind the partition, respectively.

Let

$$\begin{pmatrix} \rho_L \\ u_L \\ p_L \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad \begin{pmatrix} \rho_R \\ u_R \\ p_R \end{pmatrix} = \begin{pmatrix} 0.125 \\ 0 \\ 0.1 \end{pmatrix}.$$
(11)

At time t = 0, the partition is instantly removed. Then the configuration splits into a rarefaction wave propagating to the left and SW with a contact discontinuity propagating to the right.

Fig. 3 presents graphs of the numerical solution to the problem (11) by various modifications of LPM, as well as the graph of the analytical solution obtained from the relations for the decay of an arbitrary discontinuity at the time t = 0.502, where the Courant net number Co = 0.3. Here dot-dash line represents the modified LPM [8], dotted line is the modified LPM [9] such that the total energy is calculated by the formula (9), solid line is the modified LPM [9] such that the total energy is calculated by the formula (6), dashed line is the analytical solution.



Fig. 3. Solution to the problem (11) at the time t = 0.502, Co = 0.3

Fig. 4 shows a fragment of pressure graphs, which contains a SW. The graphs were obtained in the solution to the problem (11) by various modifications of LPM. All notations in Fig. 4 coincide with the notations in Fig. 3.



Fig. 4. Solution to the problem (11). SW is at the time t = 0.502, Co = 0.3

Fig. 3 and 4 show that the obtained numerical solutions coincide with the analytical solution as a whole. The only exception is the modified LPM [9] such that the total energy is calculated by the formula (9). As noted above, the calculation by this modification involves the fact that the specific total and internal energies at the shock change are overestimated and the density is underestimated. In addition, the shock front exceeds the analytical solution. Also, in contrast to [8], oscillations at the front of the vacuum wave are not observed. At the front of the SW, the oscillations of the modified method are significantly less than the oscillations of the basic method. The solution to the problem (11) obtained by the modified method is stable with Courant numbers up to Co = 0.85. In the case of solving the problem (11) by the basic LPM, the calculation fails, if the Courant grid number is more than Co = 0.7. Note that the authors of the paper [8] obtained a solution for the decay of an arbitrary discontinuity by modified LPM up to Co = 1.1. However, the authors solved another problem.

Then, we solve the problem (11) by the modified LPM such that the density is recalculated at the Euler stage using the formula (9) and by the basic LPM using artificial pseudo-viscosity in the form (4). Fig. 5 shows the results of calculations for the Courant net number Co = 0.3 and time t = 0.502.



Fig. 5. Solution to the problem (11) at the time t = 0.502, Co = 0.3: solid line represents the basic LPM with pseudo-viscosity(4), dot-dash line is the modified LPM with recalculation of the density, the dashed line is the analytical solution

If pseudo-viscosity is included in the basic method, then the front of the SW remains behind the analytical solution (Fig. 5). In this case, the pressure on the contact discontinuity is overestimated. The position of the rarefaction wave qualitatively coincides with the analytical solution.

The use of density recalculation at the Euler stage proposed in [9] led to a strong advance in the fronts of compression and rarefaction waves. The pressure at the contact discontinuity also turned out to be overestimated.

# Conclusion

Analysis of the solutions to test problems by various modifications of the LPM showed the following features.

– If pseudo-viscosity is included in the basic LPM, then the front of the SW remains behind the analytical solution, and the pressure on the contact discontinuity is overestimated.

– If the density is recalculated at the Euler stage, then the numerical solution does not coincide with the analytical solution.

- The solution obtained by the modified LPM [8] best coincides with the analytical solution to the problem on the decay of an arbitrary discontinuity.

There are the following advantages of the modified LPM described in [8]: a significant decrease in the oscillations at the front of the SW in comparison with the classical LPM, a wider range of the Courant grid number obtained without complicating the basic algorithm.

The proposal to specify density [9] is interesting from the theoretical and practical points of view, but the proposal requires further study.

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# АНАЛИЗ НЕКОТОРЫХ МОДИФИКАЦИЙ МЕТОДА КРУПНЫХ ЧАСТИЦ ДЛЯ МОДЕЛИРОВАНИЯ ЗАДАЧ ВОЛНОВОЙ ДИНАМИКИ

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В данной работе был проведен численный анализ различных модификаций метода крупных частиц применительно к задачам волновой динамики (газовой динамики). С помощью модификаций метода крупных частиц были решены задачи расчета распада произвольного разрыва, распространение ударных волн и распространения волн разрежения. Расчеты распространения стационарных ударных волн показывают, что все модификации метода крупных частиц правильно позволяют рассчитывать давления за ударной волной, несмотря на различия по ширине зоны ударного перехода и профиля давления ударной волны в этой зоне в зависимости от модификации метода крупных частиц. При решении задачи о распаде произвольного разрыва было показано, что модификация метода крупных частиц с пересчетом давления на эйлеровом этапе, наилучшим образом совпадает с аналитическим решением задачи о распаде произвольного разрыва, как в области ударной волны, так и в области волны разрежения. Значительным достоинством данной модификации является тот факт, что рассмотренные в работе задачи могут быть решены без введения в законы сохранения «искусственной» вязкости.

Ключевые слова: ударная волна; распад произвольного разрыва; число Куранта; искусственная вязкость; крупные частицы.

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