ON ONE METHOD OF CALCULATING MOVING BOUNDARIES IN EULER COORDINATES

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The paper presents a method for calculating a moving boundary in Euler coordinates as an application to studies of gas flows in areas with an impermeable wall. The method is based on a combination of the Eulerian grid and one Lagrangian border cell formed by the combination of two cells adjacent directly to the moving border. Reconstruction of the entire computational domain is not required. This fact has a significant impact on the computational performance. We describe the algorithm for combination of cells, present the calculation of thermodynamic parameters, and justify the expression for the internal energy of the combined interval. The method was verified using an analytical solution to the problem of a converging shock wave in a vessel with an impermeable wall. Finally, we compare the entropy functions of the analytical and numerical solutions.

Keywords: numerical method; moving boundary; Euler coordinates; method of large particles; converging shock wave.

Introduction

Liquid and gas flows with moving boundaries are widespread in various technological processes and are of great importance in industry. The following several types of devices can be distinguished: high-speed explosive closures designed to shut off steel pipelines in the nuclear, oil, and gas industries [1]; conservation ampoules used to obtain new materials (compaction of metal or ceramic powders by shock waves) [2]; explosion-proof chambers designed to localize the effects of the explosion; ammunition of fragmentation and cumulative principles of action [3, 4]. The work of many gas-dynamic devices is often associated with the deformation of the working body, which in most cases is made of metal and has a shape close to plane, cylindrical or spherical. Under such a specific effect as shock-wave loading, the study of dynamic processes in spherical and cylindrical shells is a complex and actual problem. Along with studies of processes occurring in shells under radial compression, it is equally important to study processes occurring during radial tension, which are realized when shells expand under the action of explosive loads.

In experiments, the shell is deformed under the action of explosion product located on its outer surface. In the ideal case, an uniformly distributed load impulse compresses all shell elements to the axis of symmetry with the same initial velocity until all kinetic energy is expended on the work of elastic and plastic deformation. Therefore, as a result of the radial deformation of the shell, we obtain a shell with smaller external and internal radii and a larger thickness.

An experimental study of such problems involves considerable difficulties and costs. Therefore, an actual problem is the development of physical and mathematical models and a numerical algorithm that can reliably describe the flow of a liquid or gas with moving impermeable boundaries.
In the overwhelming majority of cases, Lagrangian methods are used for such problems [5, 6]. Namely, the cells of the computational grid move together with the liquid and, therefore, there is no need to select contact boundaries in a special way. However, with sufficiently considerable deformations of the substance, there is a strong distortion of the grid cells, which causes a decrease in both the accuracy of calculations and the time step. And in some cases, there is a loss of the metric proximity of neighboring nodes of the Lagrangian grid. These shortcomings are removed by using the algorithms that support the convexity of cells, uneven grids, or the procedure of reconstruction of a grid [7].

In the Euler methods [5, 8], the nodes of the computational grid are fixed and do not change during the calculation. As a result, flows with considerable deformations can be investigated. In order to construct grids that take into account the shape of the boundaries of the computational domain or its mobility, one can use methods of constructing adaptive grids, where there are moving grids that are rigidly connected with the movement of the boundary [9-13]. However, such methods lead to a significant complication of the computational algorithm and an increase in the computational time.

There exists a number of Lagrangian – Euler methods that use a combination of the Lagrangian and Euler grid [14]. In this paper, we propose a modification of the method [15] based on a combination of the Eulerian grid and one Lagrangian boundary cell formed by the union of two cells adjacent directly to the moving boundary. Therefore, the main calculation is carried out on an Eulerian grid, and the reconstruction of boundary cells does not require large expenditures of computer time. In contrast to [15], we propose to calculate the internal energy of the combined interval instead of the total energy. The proposed approach does not lead to oscillations of the solution at the boundary. The method is also generalized to the case of cylindrical and spherical symmetry in the one-dimensional case. Let us show the essence of the method by the example of such a modification of the Harlow method as the method of large particles (MLP) [8].

1. Method of Large Particles

The main idea of the MLP is to split the system of Euler equations according to physical processes [8]. At each time step, the values are calculated in three stages. Let us briefly describe the MLP in the one-dimensional case and the changes associated with the generalization for all types of symmetry.

Consider the movement of an ideal liquid in the one-dimensional case. As the initial equations, we take the Euler differential equations in divergent form (the equations of continuity, momentum, and energy):

\[ \frac{\partial \rho}{\partial t} + \text{div}(\rho v) = 0 \]  \hspace{1cm} (1.1)

\[ \frac{\partial \rho v}{\partial t} + \text{div}(\rho vv) = -\text{grad}(p) \]  \hspace{1cm} (1.2)

\[ \frac{\partial \rho E}{\partial t} + \text{div}(\rho Ev) = -\text{div}(pv). \]  \hspace{1cm} (1.3)

Here \( \rho \) is the density, \( E = \varepsilon + 0.5v^2 \) is the total specific energy, \( \varepsilon \) is the internal energy, \( p \) is the pressure, \( v \) is the velocity. In order to close system (1.1)–(1.3), we use the equation
of state of an ideal gas in the following form:

\[ p = (\gamma - 1)\rho \varepsilon, \]

where \( \gamma \) is the adiabatic exponent.

The first stage, i.e. the Euler stage, involves neglecting all the effects associated with the movement of the unit cell (there is no mass flow through the cell boundaries), and takes into account only the effects of liquid acceleration due to pressure. At this stage, intermediate values of velocity and energy of the flow are determined [8]. Taking into account these assumptions, we obtain that the terms of the equations having the form \( \text{div}(\varphi \rho v) \), where

\[ \varphi = (1, v, E), \]

are taken equal to zero. Then, it follows from the continuity equation that \( \rho = \text{const} \), therefore, in the remaining equations, the density can be taken out from under the differential sign:

\[ \rho \frac{\partial v}{\partial t} = -\text{grad}(p) \quad (1.4) \]

\[ \rho \frac{\partial E}{\partial t} = -\text{div}(pv). \quad (1.5) \]

Write equations (1.4)–(1.5) in the general case for plane, cylindrical, and spherical symmetry:

\[ \rho \frac{\partial v}{\partial t} + \frac{\partial p}{\partial r} = 0 \quad (1.6) \]

\[ \rho \frac{\partial E}{\partial t} + \frac{1}{r^{\alpha-1}} \frac{\partial}{\partial r} r^{\alpha-1} pv = 0, \quad (1.7) \]

where \( \alpha \) is the type of symmetry. Namely, the equations describe movements with plane, cylindrical, and spherical symmetry, for \( \alpha = 1, \alpha = 2, \) and \( \alpha = 3, \) respectively.

Now we consider the finite-difference approximations of the first order of equations (1.6)–(1.7) at the time \( t^n \):

\[ \tilde{v}_i = v_i - \frac{p^n_{i+1/2} - p^n_{i-1/2}}{\Delta t} \rho^n_i \frac{\Delta t}{\Delta r} \]

\[ \tilde{E}^n_i = E^n_i - \frac{1}{(r^n_i)^{\alpha-1}} \frac{(r^n_{i+1/2})^{\alpha-1} p^n_{i+1/2} v^n_{i+1/2} - (r^n_{i-1/2})^{\alpha-1} p^n_{i-1/2} v^n_{i-1/2}}{\Delta t \rho^n_i}, \quad (1.8) \]

where \( r_i \) is the coordinate of the center of the \( i \)-th cell at the time \( t^n \). The quantities \( \varphi = (v, p, r) \) with fractional indices are considered to be related to the cell face and are determined as follows:

\[ \varphi^n_{i+1/2} = \frac{\varphi^n_i + \varphi^n_{i+1}}{2}. \quad (1.9) \]

At the second stage, i.e. the Lagrangian stage, we calculate mass flows through the boundaries of the Euler cells. Formulas for calculating mass flows follow from continuity equation (2.1), which, as a result of approximation, takes the form

\[ \frac{\rho_{i+1}^n - \rho_i^n}{\Delta t} + \frac{1}{(r^n_i)^{\alpha-1}} \frac{(r^n_{i+1/2})^{\alpha-1} \rho^n_{i+1/2} \tilde{v}_i^n - (r^n_{i-1/2})^{\alpha-1} \rho^n_{i-1/2} \tilde{v}_i^n}{\Delta r} = 0. \quad (1.10) \]
Rewrite (1.11) in the form
\[
\rho_i^{n+1}(r_i)^{a-1} \Delta r = \rho_i^n(r_i)^{a-1} \Delta r - \Delta M_i^{n+1/2} + \Delta M_i^{n-1/2},
\]
(1.12)
where
\[
\Delta M_i^{n+1/2} = (v_{i+1/2}^n)^{a-1} < \rho_{i+1/2}^n > < \tilde{v}_{i+1}^n > > \Delta t.
\]
(1.13)
The quantities given in angle brackets are considered to be set at the cell boundary. In this paper, in order to calculate the mass flow, we use the first-order formulas taking into account the flow direction:
\[
\Delta M_i^n = \begin{cases} 
\rho_i^n \frac{v_i^n + v_{i+1}^n}{2} (r_i^n)^{a-1} \Delta t, & \tilde{v}_i^n + \tilde{v}_{i+1}^n > 0 \\
\rho_i^n \frac{v_i^n + v_{i+1}^n}{2} (r_i^n)^{a-1} \Delta t, & \tilde{v}_i^n + \tilde{v}_{i+1}^n < 0.
\end{cases}
\]

At the third stage, i.e. the final stage, the final values of the parameters \( \rho, X = (v, E) \) in the cell are calculated by the formulas obtained from (1.12):
\[
\rho_i^{n+1} = \rho_i^n + \frac{\sum \Delta M_i^k}{(r_i)^{a-1} \Delta r}, \quad X_i^{n+1} = X_i^n + \frac{\sum \tilde{X}_i^k \Delta M_i^k}{\rho_i^{n+1}(r_i)^{a-1} \Delta r}.
\]

2. Method for Calculating the Moving Boundary

The algorithm for calculating the moving boundary is based on the representation of the boundary cell as Lagrangian-Euler one [15]. Obviously, movement of the boundary involves a compression of the cell, which leads to a decrease in the time step, and when, under compression to an infinitely small value, leads to a loss of stability of the method. In order to solve this problem, it is advisable to combine two cells adjacent to the moving boundary into one cell. Therefore, the combined cell is larger than the remaining cells of the Eulerian grid, and this fact does not affect the stability of the method. As soon as the size of the combined cell reduces to the size of the minimum cell of the main Eulerian grid when the boundary is moved, the cell is combined with the next one, etc. The procedure of combination of cells is advisable to carry out before the Euler stage.

Consider the relations for obtaining new parameters of the combined cell in the general case, when the cell sizes are not equal. Calculate the lengths of the intervals by the following formulas [16]:
\[
\Delta r_L = \frac{s_\alpha}{\alpha} ((r_{i-1})^\alpha - (r_i)^\alpha), \quad \Delta r_R = \frac{s_\alpha}{\alpha} ((r_i)^\alpha - (r_{i+1})^\alpha), \quad \Delta r_C = \Delta r_R + \Delta r_L,
\]
where
\[
s_\alpha = \begin{cases} 
1, & \alpha = 1 \\
2\pi, & \alpha = 2 \\
4\pi, & \alpha = 3
\end{cases},
\]
the indices \( \langle L \rangle, \langle R \rangle, \) and \( \langle C \rangle \) correspond to the left, right, and combined cell, respectively. Then the masses, momenta, and energies of these intervals are as follows:
\[
\Delta M_L = \rho_L \Delta r_L, \quad \Delta K_L = v_L \Delta M_L, \quad \Delta Q_L = E_L \Delta M_L.
\]
\[
\Delta M_R = \rho_R \Delta r_R, \quad \Delta K_R = v_R \Delta M_R, \quad \Delta Q_R = E_R \Delta M_R.
\]
Denote the mass concentrations of the intervals $\Delta M_R$ and $\Delta M_L$ in the combined interval by $\xi_L$ and $\xi_R$, where $\xi_L = \Delta M_L / (\Delta M_L + \Delta M_R)$, $\xi_R = \Delta M_R / (\Delta M_L + \Delta M_R)$.

The mass concentrations $\xi_L$ and $\xi_R$ satisfy the condition

$$\xi_L + \xi_R = 1. \tag{2.1}$$

The values of the density, velocity, and specific total energy of the combined cell are found by the laws of conservation of mass, momentum, and energy:

$$\rho_C = (\Delta M_L + \Delta M_R) / \Delta r_C, \tag{2.2}$$
$$v_C = (\Delta K_L + \Delta K_R) / (\Delta M_L + \Delta M_R), \tag{2.3}$$
$$E_C = (\Delta Q_L + \Delta Q_R) / (\Delta M_L + \Delta M_R). \tag{2.4}$$

Let us consider the change in kinetic energy during the transition from the quantities determined for the intervals $\Delta M_R$ and $\Delta M_L$ to the quantities determined for the combined interval $\Delta M_R + \Delta M_L$. The sum of the kinetic energies of the intervals $\Delta M_R$ and $\Delta M_L$ is equal to

$$\bar{\bar{Q}} = 0.5 \left( v_R^2 \Delta M_R + v_L^2 \Delta M_L \right). \tag{2.5}$$

The kinetic energy of the combined interval is determined by its velocity $v_C$ according to the formula

$$Q_C = 0.5v_C^2 (\Delta M_R + \Delta M_L). \tag{2.6}$$

Excess kinetic energy

$$\Delta Q = \bar{\bar{Q}} - Q_O \tag{2.7}$$

is transformed to internal energy. Let us show that this excess kinetic energy is always positive. Substitute (2.5) and (2.6) into (2.7). As a result, we obtain

$$\Delta Q = 0.5 \left( v_R^2 \Delta M_R + v_L^2 \Delta M_L - v_C^2 (\Delta M_R + \Delta M_L) \right).$$

Transform the expression $\Delta Q$ as follows. Factor out $\Delta M_R$ and $\Delta M_L$ and substitute expression of $v_C$ in terms of the velocities of the intervals $\Delta M_R$ and $\Delta M_L$:

$$v_C = v_R \xi_R + v_L \xi_L. \tag{2.8}$$

Using (2.8), we rewrite $\Delta Q$ in the form

$$\Delta Q = 0.5 \left( \Delta M_R + \Delta M_L \right) \left( v_R^2 \xi_R + v_L^2 \xi_L - v_C^2 (v_R \xi_R + v_L \xi_L) \right). \tag{2.9}$$

Transform the expression in the bracket by adding the following quantity equal to zero:

$$A = - v_C (v_R \xi_R + v_L \xi_L) + v_C^2 (\xi_R + \xi_L).$$

Indeed, this quantity is equal to zero by virtue of (2.1) and (2.8). Finally, the value of excess kinetic energy takes the form

$$\Delta Q = 0.5 \left( \Delta M_R + \Delta M_L \right) \left( \xi_R (v_R - v_C)^2 + \xi_L (v_L - v_C)^2 \right).$$
The internal energy of the combined interval \( \Delta M_R + \Delta M_L \) consists of the sum of the internal energies of the intervals \( \Delta M_R \) and \( \Delta M_L \) and the excess kinetic energy

\[
\epsilon_C (\Delta M_R + \Delta M_L) = \epsilon_R \Delta M_R + \epsilon_L \Delta M_L + \Delta Q. \tag{2.10}
\]

Substitute \( \Delta Q \) in (2.9) and divide by \( \Delta M_R + \Delta M_L \). Then, the expression for the internal energy of the combined interval takes the form

\[
\epsilon_C = \xi_R \left( \epsilon_R + 0.5(v_R - v_C)^2 \right) + \xi_L \left( \epsilon_L + 0.5(v_L - v_C)^2 \right).
\]

The pressure is found by \( \rho_C, \epsilon_C \) and the equation of state.

Generally speaking, the applied method is a method of transferring (recalculating) quantities from one spatial (old) grid to another (new, not necessarily Euler) grid. Suppose that the cell of the «new» grid of size \( r \) contains \( N \) intervals of the «old» grid in which the solution has already found, that is, the values \( \Delta r_k, \rho_k, v_k, P_k, \xi_k \) are known. Let us write the formulas in general form. It is important that the values \( \Delta r_k \) satisfy the condition

\[
\Delta r = \sum_{k=1}^{N} \Delta r_k.
\]

The masses of the intervals of the «old» grid and the mass of the interval of the «new» cell are determined using the equations

\[
\Delta M_k = \rho_k \Delta r_k, \quad \Delta M = \sum_{k=1}^{N} \Delta M_k.
\]

Then volumetric and mass concentrations are as follows:

\[
\alpha_k = \frac{\Delta r_k}{\Delta r}, \quad \xi_k = \frac{\Delta M_k}{\Delta M}. \tag{2.11}
\]

It follows from (2.10) that \( \alpha_k \) and \( \xi_k \) satisfy the conditions:

\[
\sum_{k=1}^{N} \alpha_k = 1, \quad \sum_{k=1}^{N} \xi_k = 1.
\]

The laws of conservation of mass, momentum, and energy involve the following equations for determining the average values in the new cell:

\[
\rho = \sum_{k=1}^{N} \alpha_k \rho_k, \quad v = \sum_{k=1}^{N} \xi_k v_k, \quad \varepsilon = \sum_{k=1}^{N} \xi_k \left( \varepsilon_k + 0.5(v_k - v)^2 \right).
\]

Pressure is determined by the equation of state.

As soon as the size of the combined cell is reduced to the size of the minimum cell of the main Eulerian grid, the cell is combined with the next one, etc. At each time step before the Eulerian stage begins, the parameters of the combined (Lagrangian) cell are recalculated according to the formulas for the isentropic flow, when the moving boundary is moved:

\[
\rho_{Cb} = \rho_{Ca} \left( \frac{\Delta r_{Cb}}{\Delta r_{Ca}} \right)^\alpha, \quad u_{Cb} = \rho_{Ca} u_{Cb} \left( \frac{\Delta r_{Cb}}{\Delta r_{Ca}} \right)^\alpha = u_{Cb},
\]

\[
p_{Cb} = p_{Cb} \left( \frac{\rho_{Ca}}{\rho_{Cb}} \right)^\gamma = p_{Cb} \left( \frac{\Delta r_{Ca}}{\Delta r_{Cb}} \right)^\gamma, \quad \varepsilon_{Ca} = \varepsilon (\rho_{Ca}, p_{Ca}), \quad E_{Ca} = \varepsilon_{Ca} + \frac{u_{Ca}^2}{2},
\]

where the indices «b» and «a» denote the parameters of the combined cell before and after compression, respectively.

Therefore, this algorithm for reconstruction of grid only affects the cells adjacent to the moving boundary, without requiring reconstruction of the entire computational domain. This fact has a positive effect on the computational performance.
3. Verification of the Method

In order to evaluate the accuracy of the developed method, we use an analytical solution to the problem of a converging shock wave in a vessel with an impermeable wall, which describes cases of plane, cylindrical, and spherical symmetry [17]. Consider a vessel with an impermeable wall of size $r_0 = 1$, in which there is a gas with the initial parameters $\rho_0 = 1$, $v_0 = 0$, $P_0 = 0$, $\varepsilon_0 = 0$, $\gamma = 5/3$. At the initial moment of time, the velocity $v_{00} = -1$ is set at the boundary. At several points in time, the profiles of pressure, velocity, density, and entropy function are shown in Figs. 1–3.

![Fig. 1. Profiles of pressure (A), velocity (B), density (C), and entropy function (D) at three points in time: 1 at $t = 0, 4$; 2 at $t = 0, 45$; 3 at $t = 0, 5$ for the spherical case. Here the solid and dotted lines denote the analytical and numerical solutions, respectively.](image)
Fig. 2. Profiles of pressure (A), velocity (B), density (C), and entropy function (D) at three points in time: 1 at $t = 0.45$; 2 at $t = 0.525$; 3 at $t = 0.6$ for the cylindrical case. Here the solid and dotted lines denote the analytical and numerical solutions, respectively.
Fig. 3. Profiles of pressure (A), velocity (B), density (C), and entropy function (D) at three points in time: 1 at $t = 0.5$; 2 at $t = 0.6$; 3 at $t = 0.7$ for the plane case. Here the solid and dotted lines denote the analytical and numerical solutions, respectively. The values $\Delta P$, $\Delta v$, $\Delta \rho$, $\Delta F$ are fictitious and introduced to improve the readability of the graphs.

The numerical and exact solutions are compared for the three types of symmetry. The profiles of pressure, velocity, and density are consistent with the analytical solution. The graphs of density show a small entropy trace. However, a comparison of the entropy functions shows that the relative deviation of the calculated value of the function from the exact is not more than 0.01% maximum behind the shock wave front.
Conclusions

The paper presents a method for calculating liquid and gas flows in the presence of a moving boundary in the computational domain in Euler coordinates. The method was verified using an analytical solution to the problem of a converging shock wave in a vessel with an impermeable wall. We show a good convergence of the numerical solution to the analytical one. The proposed method for calculating the thermodynamic parameters of the combined interval does not lead to oscillations of the solution at the boundary. Therefore, the developed software package can be used for numerical simulation of dynamic processes in shells.

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ОБ ОДНОМ МЕТОДЕ РАСЧЕТА ПОДВИЖНЫХ ГРАНИЦ В ЭЙЛЕРОВЫХ КООРДИНАТАХ

Е. С. Шестаковская, Я. Е. Стариков

В работе приводится метод расчета подвижной границы в эйлеровых координатах в приложении к исследованиям течений газа в областях с непроницаемой стенкой. Метод основан на комбинации эйлеровой сетки и одной лагранжевой приграничной ячейки, образованной объединением двух ячеек, прилегающих непосредственно к подвижной границе. Перестройка всей расчетной области не требуется, что оказывает существенное влияние на производительность расчетов. Изложен алгоритм объединения ячеек, расчет термодинамических параметров и обоснование выражения для внутренней энергии объединенного интервала. Проведена верификация метода с помощью аналитического решения задачи о сходящейся ударной волне в сосуде с непроницаемой стенкой. Проведено сравнение энтропийных функций аналитического и численного решений.

Ключевые слова: численный метод; подвижная граница; эйлеровы координаты; метод крупных частиц; сходящаяся ударная волна.

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