Meshfree Particle Method Using Molecular Dynamics Techniques for Simulating Viscous Compressible Flows

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Abstract. The work to improve and expand of capabilities of the meshfree particle methods by using molecular dynamic simulations approaches was carried out. The theoretical background and methodological basis of the modified technique, computational aspects and software implementation, as well as examples of application of the proposed hybrid technology for solving actual applied problems are described.

1. Introduction

With the rapid development of computer technologies and software, computational simulation has become of paramount importance for solving modern engineering and scientific problems. Numerical modeling is a widely applied technique to confirm theories, to understand, interpret and even predict complex physical phenomena. Grid-based approaches, like the finite difference method (FDM) [1 – 6], the finite element method (FEM) [7 – 10] and the finite volume method (FVM) [11, 12], are the most common choices for integrating of model partial differential equations (PDEs).

The finite difference method [1 – 6] is one of the earliest and widely used methods for solving the equations of continuum mechanics. This approach does not require large computational resources and gives fairly accurate Taylor series approximations of differential equations. An essential disadvantage of FDM is the inapplicability of this method in computational domains with nontrivial geometry. The complexity, or even impossibility, to transforming the initial domain to a simple configuration significantly narrows the range of problems that can be solved by FDM technique. The latter circumstance made it imperative to develop new and more universal approaches, such as the finite element method [7 – 10] and the control volume method (finite volume method) [11, 12]. These methods allow to solve complex engineering problems in arbitrary computational domains.

The concept of the FEM [7 – 10] is based on the domain discretization into a collection of finite-size elements and the piecewise continuous approximation of the unknown functions (temperature, pressure, velocity, etc.). The piecewise polynomials are frequently employed for approximating functions that are equal to zero outside the corresponding finite element. Moreover, the basic functions must satisfy the conditions of equality of their values on the common boundaries of adjacent elements and the imposed boundary conditions. The coefficients of the approximating functions are expressed in terms of unknown solution values at nodes. The governing partial differential equations are replaced by a system of algebraic equations, the number of which corresponds to the number of unknowns at the grid nodes. The solution to the problem is the function values at the vertices of the mesh partition.

The control volume method [11, 12] uses the integral formulation of conservation laws include conservation of energy, conservation of momentum, conservation of mass, etc. The discrete analogues of the equations are obtained on the basis of balance ratios by summing of energy, mass and
momentum fluxes through the all surfaces of the control volume. This formulation does not impose restrictions on the shape of the control volume, allows use of both structured and unstructured grids with different cell shapes and solves the complex geometry problem.

These grid-related methods use two different Lagrangian and Eulerian representations of fluid flow [13]. The Eulerian approaches (which include FDM and FVM methods) are built on the basis of a fixed grid in space. A continuous medium moves through the fixed computational cells, and the mass, momentum and energy fluxes through the grid cells boundaries are calculated in order to find the distributions of parameters in the computational domain. The methods based on the Eulerian description are not sensitive to large deformations of medium, since the computational grid remains stationary. Thus, these approaches are successfully used to solve gas dynamic problems with high accuracy. However, this group of techniques has a number of significant drawbacks. First, there is no way to trace the history of flow field change in the chosen microvolume, the motion of which cannot be traced using a stationary Eulerian grid. The method gives an overview of the changing the parameter field in fixed grid nodes. Secondly, accurate boundary condition assignment at deformable free surfaces and phase boundaries, whose position is not known in advance, is problematic.

In the Lagrangian description used by FEM, the discrete elements are frozen into the moving medium and carry out a transfer of mass, momentum and energy. In this case, the mass of each element remains unchanged, that allows to not calculate the fluxes of mass across the cell boundaries. The latter circumstance enables to eliminating convective components of differential equations, greatly simplify the program code and give a significant gain in productivity. The Lagrangian computational methods are simple to program implementation and allow to easily satisfy the boundary conditions on free surfaces and moving phase separation boundaries, which are determined by the positions of boundary nodes of deformable mesh. Thanks to the above advantages, classical Lagrangian methods using approximation on a Lagrangian grid are widely applied in computational solid mechanics, where the deformations are not so large compared with those that occur during computational gas dynamics modeling. However, this class of approaches has a significant drawback: the accuracy of numerical solutions is considerably reduced in the presence of strong deformations, medium distortions and, consequently distortions of the computational grid, which is rigidly connected with it. In addition, the time step, which is determined by the smallest cell size, can become too small leading to unacceptable slow down the calculation process or even crash the solution. This circumstance makes it necessary to periodic rebuild the computational grid and subsequent interpolation, which is a rather laborious process leading to an increase in the computational error.

The tempting prospect of using combined approaches that make it possible to take advantages of both descriptions and to level out their shortcomings has led to the creation of mixed methods based on both Lagrangian and Eulerian representations of fluid flow.

The Particles-In-Cell method (PIC) [14, 15] was developed in the Los Alamos laboratory in the middle 1950s to calculate processes with large deformations. This technique uses a fixed Eulerian grid and a set of mobile Lagrangian particles which move through the grid. The implementation of the method includes the Eulerian and Lagrangian steps. At the first stage, in the assumption that effects associated with a mass transport through the cell boundaries are negligible, the intermediate values of the sought flow parameters are determined, taking into account the gas acceleration only due to pressure difference. At the Lagrangian stage, the particle flux across the boundaries of the Eulerian grid cells is calculated. In so doing, it takes into account the contribution of the convective components. The particles-in-cell method has allowed to essentially increase the range of problems which can be solved using PIC and to simulate multiphase flows at very large deformation of interfaces or free surfaces. At that time, however, computers could not provide the necessary performance to use a sufficient number of Lagrangian particles. The latter circumstance led to low-accuracy solutions with significant oscillations of flow parameters that promoted the development of more economic methods.
The Method of Large Particles (MLP) [16–19] is a development of the particles-in-cell method. The main difference between the two technologies is that the MLP implies a calculation of the mass flux across cell boundaries, instead of modeling of the Lagrangian particles displacements.

A method proposed and developed in [20–22] is based on an Arbitrary Lagrangian–Eulerian (ALE) description of complex nonstationary processes. The method uses a mobile grid which motion is not related to the movement of the medium. The approach consists in moving, local rebuilding the grid in areas with large deformations and subsequent interpolation of data on a new grid. This technology is often used to simulate the motion of bodies immersed in a liquid. The main disadvantages of the method are: low efficiency, blurring of the flow pattern, a considerable decrease in the solution accuracy due to the use of a resource-intensive interpolation procedure. In addition, the mutual overlapping of the computational cells can occur in the computational simulation of moving interfaces or free surfaces.

Despite their great success and wide distribution, grid methods have significant disadvantages that limit their application in many nontrivial cases, such modeling of free surface flows with large deformations and inhomogeneities, deformable mobile phase interfaces, high-speed processes in medium and solving a number of astrophysical problems. The main difficulties are related to domain partitioning with a computational grid. Mesh generation is central to the whole concept of grid methods. At the same time, the quality of complex grid models must satisfy a number of stringent criteria. The implementation of these requirements is necessary for the effective application of the numerical techniques and the provision of specified accuracy. Experience shows that when solving applied problems the creation of high-quality adaptive grids with significant refinement in the large gradient regions requires more time resources than the computational process. The presence of rigid topological connections between the nodes makes the grid adaptation procedure difficult and can lead to self-intersection of the elements. This is especially the case in Lagrangian grid approaches.

The use of gridless Lagrangian techniques makes it possible to fully utilize the advantages of Lagrangian approaches and to avoid problems associated with computational grids. Thanks to the rapid development of computer technologies and the continuous expansion of computing power, in the short term, the alternative gridless methods will be able to compete with the traditional approaches in many areas. The universality of the technique makes it possible to use it in the modeling of the widest range of physical phenomena and systems in the context of discrete or continuous medium models, in scales from the microworld to the entire Universe, and for solving practically important engineering problems. Meshless methods can be successfully applied both in the fields of computational gas dynamics and computational solid mechanics for the needs of the aviation, rocket, space, nuclear, energy, chemical, oil and gas, medical and pharmaceutical industries in various spheres of production.

The monograph [23] gives an extensive review of the existing gridless methods, which development was constrained by the limitations of computational resources for more than a decade. Modern high performance computing technologies based on GPUs (graphics processing units) provide significant opportunities for these methods in achieving a new level of accuracy, reliability and applicability, including their wide use in commercial gasdynamic software packages.

The most well-known among the meshless Lagrangian approaches is the Smoothed Particle Hydrodynamics (SPH) method. The SPH method was first proposed in [24, 25] for describing astrophysical phenomena. Later, thanks to the works [26–29], it was extended to solve a wide range of problems of solid mechanics [30–32], dynamics of multiphase media [33–35] and magnetic hydrodynamics [28, 36]. To date, a significant number of its variations have been created. These modifications differ in the smoothing functions, approaches to discretization of the governing equations and other implementation details. The smoothed particle hydrodynamics method is adapted for calculation turbulent flows [37], solving problems of relativistic mechanics [38, 39], modeling underwater explosions [40, 41] and flows through porous materials [42, 43], etc.

The SPH method is based on two assumptions. First, the simulated medium is represented by a system of moving particles, which are located at certain points in the space of the computational domain at a given moment. Particles are endowed with physical properties, such as mass, internal
energy, velocity, temperature, density, etc. Secondly, each particle has a radius and so-called smoothing length.

The physical parameters in the closest region that is bounded by the particle radius are determined by the smoothing function, often called smoothing kernel function. Thus, the desired parameter at an arbitrary point in space can be found using known parameter values at centers of the nearest particles whose radii cover this point and corresponding values of smoothing functions. The action of the latter is limited by the particle radius.

Although traditional grid-based techniques, such as FDM, FEM and FVM, remain the dominant in computational fluid dynamics and computational solid mechanics, the meshless methods are a very promising alternative to the classical approaches in solving a wide range of practically important problems. The gridless methods are more versatile and can be used not only for modeling of continuous media, but also for the numerical description of discrete systems include, for example, the interaction of stars in astrophysics, the motion of billions of atoms, the dynamic behavior of complex protein molecules. New generation of computational methods make it possible to obtain stable and high precision numerical solutions of integral equations or partial differential equations with all possible boundary conditions using a set of optimally distributed nodes (particles) without applying the grid that connects them. Therefore, the task of developing the gridless methods with the aim of improving the approximation characteristics, increasing efficiency and stability, and expanding the scope of their application, is extremely urgent.

The present study is devoted to the improvement and the expansion of capabilities of the meshfree particle methods by using molecular dynamic simulations approaches. The paper describes the theoretical background and methodological basis of the modified technique, computational aspects and software implementation, as well as examples of application of the proposed hybrid technology for solving actual applied problems.

2. Mathematical description of the modified meshless particle method for modelling of viscous compressible flow
The modified meshless particle method uses a set of moving particles for mathematical description of the state and evolution of complex physical systems. Particles can be used both for describing the individual elements of a discrete system and for representing a continuous medium from micro- to macro-scales. Each particle locates at a certain point in the space of the computational domain and possesses mass, internal energy, velocity, temperature, density, etc.

Let us consider the motion of a continuous medium in the case of the two-dimensional computational domain. At each moment in time, the state of a system under investigation is characterized by a set of distributed parameters, which are given in the form of continuous functions. In the numerical simulation, continuous functions are approximated by discrete analogs, which are defined in the instantaneous locations of moving particles. A similar approach to the approximation of functions at \( N \) points is used in Monte Carlo numerical simulation methods [44], however, the significant difference between the proposed technology and the Monte Carlo approach is that the computational nodes are not randomly generated, but are optimally distributed in the computational domain. Wherein the greater the density of nodes (particles) and the more uniform their distribution, the more accurate the approximation and, consequently, the higher the accuracy of the results.

The previous works [45 – 49] were devoted to solving the problem of optimal arrangement of nodes for an unstructured computational grid by molecular dynamics simulation, with the aim of its subsequent application in the framework of the classical grid approaches. The present approach assumes that the optimal distribution of particles in the solution domain precedes the main stage of gas dynamic modelling. It is assumed that, the most appropriate way is to locate particles in the centers of disjoint circles (or spheres) with diameters \( d_0 \) in the most-dense packing. For adaptive distribution of particles the diameters can be changed according to the desired law (for example, depending on the distance to the domain boundary).
Further realization of the method implies the integration of the Navier–Stokes (or Euler) equations of gas dynamics on a set of optimally distributed nodes. The functions and derivatives included in the system of governing partial differential equations with the corresponding boundary and initial conditions are approximated by their discrete analogs. The values of the functions and derivatives are determined in the every computational node (particle position) using information about the properties of the nearest particles which are located within its zone of influence. The region affected by the $i$-th particle is taken as its radius $R_i$, which was assumed to be equal to twice the distance to the nearest neighbour $R_i = 2 \cdot L_{\text{min}}$. Thus, the eighteen neighbours enter the influence zone of the $i$-th particle for the case of a homogeneous distribution of particles (figure 1).

The simulated medium is represented as a system of $N$ particles with mass $m$, moving at velocity $\mathbf{v}_i$. The instantaneous positions of their centres are determined by the radius vector $\mathbf{r}_i(x_i, y_i)$. Each $i$-th particle is endowed with internal energy $e_{\text{int},i}$, density $\rho_i$, pressure $p_i$, etc. The complete set of gas-dynamic parameters characterizing the state of the system under consideration is determined by the task specificity.

As noted above, every particle has a radius $R_i$ that limits its area of influence. The so-called kernel function $\phi(\mathbf{r})$ is defined in this region. This continuous function determines the degree of influence of the $i$-th node properties on parameters at an arbitrary point $j$ located inside the influence zone enclosed by a circle of radius $R_i$ (figure 2).

![Figure 1](image.png)

*Figure 1. The neighbour particle centres inside the zone of influence of the $i$-th particle with radius $R_i = 2 \cdot L_{\text{min}}$ in the case of homogeneous particle distribution.*

Suppose that some gas-dynamic variable is defined in all centers $j = 1, ..., N$ at a specific moment in time. Then, its value at an arbitrary point of the computational domain can be obtained using the weighted average approximation between the closest nodes to a given point (the so-called smoothing procedure):

$$f(\mathbf{r}^*) = \sum_{j=1}^{K} \frac{m_j}{\rho_j} \phi^*(\mathbf{r}^* - \mathbf{r}_j, R^*) f(\mathbf{r}_j),$$  \hspace{1cm} (1)$$

where $K$ is the number of $j$-th particles located in the circular region $R^*$ of influence of the test particle with coordinates $\mathbf{r}^*$; $f(\mathbf{r}_j)$ is the value of the parameter $f$ in the center of $j$-th particle placed at $\mathbf{r}_j$; $\phi^*$ is the kernel smoothing function of the test particle located at $\mathbf{r}^*$, which is not equal to zero only within the circular region of radius $R^*$. 


The definition of the kernel function $\phi_i$ for $i$-th particle.

The interpolation of function derivative $\nabla f(r^*)$ is carried out using the following relation:

$$\nabla f(r^*) = \sum_{j=1}^{K} \frac{m_j}{\rho(r_j)} \nabla \phi^*(r^* - r_j, R^*) f(r_j).$$  \hspace{1cm} (2)$$

The smoothing function is the arbitrary function satisfying the following conditions:

$$\int \phi^*(r^* - r, R^*) \, dr = 1;$$

$$\lim_{r^* \to r} \phi^*(r^* - r, R^*) = \delta(r^* - r).$$  \hspace{1cm} (3)$$

In equation (3) $\delta(r^* - r)$ is the Dirac delta function.

Mathematical model for two-dimensional, single phase, viscous, compressible perfect-gas flows, which are the objects of this research, is described by the Navier–Stokes equations in conservation law form:

$$\frac{dp}{dt} = -\rho \nabla \cdot \mathbf{v},$$  \hspace{1cm} (4)$$

$$\rho \frac{du}{dt} = -\frac{\partial p}{\partial x} + \frac{\partial \tau^{yx}}{\partial x} + \frac{\partial \tau^{yx}}{\partial y} + pF_x,$$  \hspace{1cm} (5)$$

$$\rho \frac{dv}{dt} = -\frac{\partial p}{\partial y} + \frac{\partial \tau^{xy}}{\partial x} + \frac{\partial \tau^{xy}}{\partial y} + pF_y,$$

$$\rho \frac{de_{int}}{dt} = -p\left(\frac{\partial u}{\partial x} \frac{\partial \mathbf{v}}{\partial x} + \tau^{xy} \frac{\partial u}{\partial y} + \tau^{yx} \frac{\partial v}{\partial x} + \tau^{yx} \frac{\partial v}{\partial y}\right),$$  \hspace{1cm} (6)$$

where $\rho$ is the density, $p$ is the pressure, $u, v$ are $x$- and $y$-components of the velocity $\mathbf{v}(u,v)$, $\tau^{xy} = \mu \varepsilon^{xy}$ are the components of the viscous stress tensor ($a = x,y, \beta = x,y$), $\mu$ is the coefficient of dynamic viscosity, $F_x, F_y$ are the components of the body force vector, $\varepsilon^{xy}$ are the components of the strain-rate tensor.
The equation of conservation of energy (6) is written in a simplified form because it does not take into account the process of heat transfer by conduction. The special techniques of accounting for heat conduction effects will be discussed below. The terms responsible for the viscous dissipation of energy in equation (6) with an allowance for (7) can be transformed into:

\[
\begin{align*}
\tau^{uv} \frac{\partial u}{\partial x} + \tau^{xy} \frac{\partial u}{\partial y} + \tau^{vy} \frac{\partial v}{\partial x} + \tau^{vy} \frac{\partial v}{\partial y} &= \\
= \mu \frac{\varepsilon}{3} \left( \frac{\partial u}{\partial x} + \frac{\partial u}{\partial x} - \frac{\partial v}{\partial x} - \frac{\partial v}{\partial x} \right) + \\
\mu \varepsilon^{xy} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) + \mu \varepsilon^{vy} \left( \frac{\partial v}{\partial y} + \frac{\partial v}{\partial x} \right) + \mu \varepsilon^{vy} \left( \frac{\partial u}{\partial y} + \frac{\partial u}{\partial x} \right) + \\
= \mu \varepsilon \left( e^{ux} - \frac{2}{3} \frac{\partial u}{\partial x} + \frac{2}{3} \frac{\partial v}{\partial y} \right) + \mu \varepsilon \left( e^{vy} + \frac{2}{3} \frac{\partial u}{\partial x} + \frac{2}{3} \frac{\partial v}{\partial y} \right) \tag{8}
\end{align*}
\]

Thus, the energy equation (6) is represented as follows:

\[
\begin{align*}
\frac{de_{int}}{dt} &= -p \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) + \mu \varepsilon \left( e^{ux} + e^{vy} + e^{vy} + e^{vy} + e^{vy} \right) \tag{9}
\end{align*}
\]

The governing equations (4)–(6) are closed by the defining relations for a perfect polytropic compressible gas, which are the equation of state of a perfect gas and the expression for the total energy:

\[
\rho e_{int} = \frac{p}{\gamma - 1}, \tag{10}
\]

\[
\rho e_{int} = \rho e_{int} + \rho e_{kin}, \quad \rho e_{kin} = \frac{1}{2} \rho (u^2 + v^2).
\]

In the relations (10) \( e_{int} \) is the specific total energy, which is the sum of the internal \( e_{int} \) and kinetic \( e_{kin} \) energies of the particles that form the system. The adiabatic index \( \gamma \) (the ratio of the specific heats at constant pressure and constant volume) was taken as equal to \( \gamma = c_p/c_v = 1.4 \). The speed of sound was calculated using the formula: \( c^2 = \gamma p/\rho \).

The interpretation of the meshfree particle method using molecular dynamic approaches for solving the system of equations (4)–(10) is performed as follows [26]. The density is determined from the continuity equation (4) by applying the adopted concept of particle approximation (2) [26]:

\[
\rho = \frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \frac{\partial v}{\partial y} + \frac{\partial v}{\partial y} + \frac{\partial v}{\partial y} + \frac{\partial v}{\partial y}.
\]
\[
\frac{d\rho_i}{dt} = -\rho_i \sum_{j=1}^{K} \left( \frac{m_j}{\rho_j} \right) \frac{\partial \phi_j}{\partial x_j} - \rho_j \sum_{i=1}^{K} \left( \frac{m_i}{\rho_i} \right) \frac{\partial \phi_i}{\partial y_j}. \tag{11}
\]

In the relations (11) \(K\) is the number of \(j\)-th particles located in the circular region \(R_i\) of influence of the \(i\)-th particle, \(m_j\) is the mass associated with the \(j\)-th particle, \(\phi_j = \phi(|\mathbf{r}_i - \mathbf{r}_j|, R_i)\) is the value of the \(i\)-th kernel function at the point of \(j\)-th particle location, \(\mathbf{r}_j(x_j,y_j)\) are the radius vectors of \(i\)-th and \(j\)-th particle centres, \(u_{ij} = u_i - u_j\), \(v_{ij} = v_i - v_j\) are the relative velocity components of \(i\)-th and \(j\)-th particles respectively, \(u_i, v_i, u_j, v_j\) are the velocity components.

As it follows from equation (11), the evolution of density of the \(i\)-th particle depends on its velocity relative to each of the \(j\)-th particles located in the influence region the \(i\)-th particle. In this case, the gradient of a smoothing function determines the contribution of these relative velocities.

The equations of conservation of momentum (5) in the particle approximation are treated as [26]:

\[
\frac{du_i}{dt} = -\sum_{j=1}^{K} \left( \frac{m_j}{\rho_j} \right) \frac{\partial \phi_j}{\partial x_i} + \sum_{j=1}^{K} \left( \frac{m_j}{\rho_j} \right) \left( \frac{\mu_i \varepsilon^{xx}_j}{\rho_i} + \frac{\mu_j \varepsilon^{xx}_j}{\rho_j} \right) \frac{\partial \phi_j}{\partial x_j} + \frac{p_i}{\rho_i} F_i, \tag{12}
\]

\[
\frac{dv_i}{dt} = -\sum_{j=1}^{K} \left( \frac{m_j}{\rho_j} \right) \frac{\partial \phi_j}{\partial y_i} \quad + \quad \sum_{j=1}^{K} \left( \frac{m_j}{\rho_j} \right) \left( \frac{\mu_i \varepsilon^{yy}_j}{\rho_i} + \frac{\mu_j \varepsilon^{yy}_j}{\rho_j} \right) \frac{\partial \phi_j}{\partial y_j} + \frac{p_i}{\rho_i} F_i.
\]

The components of the strain rate tensor (7) are approximated using a set of particles as follows:

\[
e^{xx}_{ij} = \frac{4}{3} \sum_{j=1}^{k} \frac{m_j}{\rho_j} u_{ij} \frac{\partial \phi_j}{\partial x_j} - \frac{2}{3} \sum_{j=1}^{k} \frac{m_j}{\rho_j} v_{ij} \frac{\partial \phi_j}{\partial y_j},
\]

\[
e^{yy}_{ij} = e^{xx}_{ij},
\]

\[
e^{xy}_{ij} = \frac{4}{3} \sum_{j=1}^{k} \frac{m_j}{\rho_j} v_{ij} \frac{\partial \phi_j}{\partial y_j} + \frac{2}{3} \sum_{j=1}^{k} \frac{m_j}{\rho_j} u_{ij} \frac{\partial \phi_j}{\partial x_j}.
\tag{13}
\]

The energy equation (6) in the framework of the adopted concept (2) is transformed into following relationship [26]:

\[
\frac{d\varepsilon_{uu.i}}{dt} = \frac{1}{2} \sum_{j=1}^{K} \left( \frac{m_j}{\rho_i} + \frac{m_j}{\rho_j} \right) u_{ij} \frac{\partial \phi_j}{\partial x_j} + \frac{1}{2} \sum_{j=1}^{K} \left( \frac{m_j}{\rho_i} + \frac{m_j}{\rho_j} \right) v_{ij} \frac{\partial \phi_j}{\partial y_j} + \frac{\mu_i \varepsilon^{xx}_i \varepsilon^{xx}_i}{\rho_i} + \frac{\mu_j \varepsilon^{xx}_j \varepsilon^{xx}_j}{\rho_j} + \frac{\mu_i \varepsilon^{xx}_i \varepsilon^{yy}_i}{\rho_i} + \frac{\mu_j \varepsilon^{xx}_j \varepsilon^{yy}_j}{\rho_j}.
\tag{14}
\]

If effects of viscosity are neglected \(\mu = 0\), then the Navier–Stokes equations reduce to the Euler equations:
\[
\frac{d\rho}{dt} = -\rho \sum_{j=1}^{K} m_j \frac{\partial \phi_i}{\partial x_j} - \rho \sum_{j=1}^{K} m_j v_j \frac{\partial \phi_i}{\partial y_j},
\]
\[
\frac{du_i}{dt} = -\sum_{j=1}^{K} m_j \left( \frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) \frac{\partial \phi_i}{\partial x_j} + \rho_i F_i,
\]
\[
\frac{dv_i}{dt} = -\sum_{j=1}^{K} m_j \left( \frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) \frac{\partial \phi_i}{\partial y_j} + \rho_i F_i,
\]
\[
\frac{de_{int,i}}{dt} = \frac{1}{2} \sum_{j=1}^{K} m_j \left( \frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) u_j \frac{\partial \phi_i}{\partial x_j} + \frac{1}{2} \sum_{j=1}^{K} m_j \left( \frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) v_j \frac{\partial \phi_i}{\partial y_j}.
\]

The presence of discontinuous solutions (shock waves), as in the case of calculation of high-speed inviscid gas flow, makes it necessary to take into account the conversion a part of kinetic energy into thermal energy when passing through a shock front. When solving the Euler equations, this process is modeled using the von Neumann–Richtmyer artificial viscous dissipation [52]. The application of artificial viscosity makes it possible to suppress nonphysical oscillations arising in the zones of high gradients of the solution. The artificial viscosity is introduced in the form proposed by Monaghan and Gingold [53].

\[
\Pi_{ij} = \begin{cases} 
-k_c \mu_i \frac{u_i + k_2 \mu_j}{\bar{\rho}_j} & \mathbf{v}_j \cdot \mathbf{r}_j < 0, \\
0 & \mathbf{v}_j \cdot \mathbf{r}_j \geq 0.
\end{cases}
\]

Here
\[
\mu_i = \frac{\mathbf{h}_i \cdot \mathbf{r}_j}{|\mathbf{r}_j|^2 + k_3 \mathbf{h}_j^2},
\]
\[
\bar{\rho}_j = \frac{\rho_i + \rho_j}{2}, \quad \bar{c}_j = \frac{c_i + c_j}{2}, \quad \bar{h}_j = \frac{h_i + h_j}{2},
\]
\[
\mathbf{v}_j = \mathbf{v}_i - \mathbf{v}_j, \quad \mathbf{r}_j = \mathbf{r}_i - \mathbf{r}_j.
\]

In the relations (17) \( c \) is the speed of sound, \( h_i = h_j = h \) is the smoothing length, \( k_1, k_2, k_3 \) are the constants. The use of artificial viscosity to compute the high-velocity gas flow over bodies can lead to excessive surface heating. This problem is solved by introducing an additional term with an artificial thermal conductivity into the energy equation [54–57]. The artificial thermal conductivities used in the form [55] and added to the energy equation:

\[
H_j = 2 \sum_{i=1}^{K} \bar{q}_{ij} \frac{e_{int,j} - e_{int,i}}{|\mathbf{r}_j|^2 + k_3 \mathbf{h}_j^2} \mathbf{r}_j \cdot \nabla \phi_i,
\]

were
\[
\bar{q}_{ij} = q_i + q_j,
\]
\[
q_i = k_i h_i \rho_i c_i \left| \nabla \cdot \mathbf{v}_i \right| + k_i h_i^2 \rho_i \left| \nabla \cdot \mathbf{v}_i \right|^2,
\]
\[
q_j = k_j h_j \rho_j c_j \left| \nabla \cdot \mathbf{v}_i \right| + k_j h_j^2 \rho_j \left| \nabla \cdot \mathbf{v}_i \right|^2.
\]

Thus, the following particle approximation of the equations of gas dynamics is used for calculating the high-speed perfect-gas inviscid compressible flows with the modified gridless method:
\[
\frac{dp_i}{dt} = -\rho \sum_{j=1}^{\kappa} \frac{m}{\rho_j} \frac{\partial \phi_{ij}}{\partial r_j}, \\
\frac{d\mathbf{u}_i}{dt} = -\sum_{j=1}^{\kappa} \frac{m}{\rho_j} \left( \frac{p_{ij}}{\rho_j^2} + \Gamma_{ij} \right) \frac{\partial \phi_{ij}}{\partial r_j} + p_i \mathbf{F}_i, \\
\frac{de_{en,i}}{dt} = \frac{1}{2} \sum_{j=1}^{\kappa} \frac{m}{\rho_j} \left( \frac{p_{ij}}{\rho_j^2} + \Gamma_{ij} \right) \mathbf{u}_j \cdot \frac{\partial \phi_{ij}}{\partial r_j} + H_i.
\]

(20)

In the present work, the third-degree piecewise spline functions (piecewise cubic splines [27]) are used to determine the kernel functions:

\[
\phi(r, h_i) = a_{3D} \times \begin{cases} 
\frac{2}{3 h_i} \left( 1 - \frac{r}{h_i} \right)^3 + \frac{1}{6 h_i} \left( 2 - \frac{r}{h_i} \right)^3 & 0 \leq r < h_i, \\
\frac{1}{6 h_i} \left( 2 - \frac{r}{h_i} \right)^3 & h_i \leq r < 2h_i, \\
0 & r \geq 2h_i.
\end{cases}
\]

(21)

Here \( r = |\mathbf{r}_i - \mathbf{r}_j | \), \( h_i = 0.5 \cdot R_i \) is the smoothing length, equal to half the particle radius \( R_i \), \( a_{3D} \) is the correction factor, which is determined by the dimension of the problem and equal to \( a_{1D} = 1/R \), \( a_{2D} = 15/(7\pi R^2) \), \( a_{3D} = 3/(2\pi R^3) \) (for one-, two- and three-dimensional cases, respectively). The graphs of the kernel function and its first derivative are shown in figure 3.

![Figure 3. The cubic spline smoothing function and its first derivative.](image)

The boundary conditions are realized by differentiating the particles. When modeling an external flow past bodies, the solid boundaries of arbitrary shape are represented using stationary particles, which are optimally distributed along the boundary [45–49]. The moving particles simulating the medium experience a repulsive force during the close approach to the boundary particles. This prevents the penetration of the medium particles beyond the “hard” boundaries of the computational domain. The Lennard–Jones pair potential, which is strongly repulsive at short distances, is used to simulate the interaction between medium and boundary particles.
In the expression (22) \( n_1, n_2 \) are the exponents accepted to be 12 and 6 respectively, \( D \) is a constant, which order is determined by the square of the maximum speed, \( d_0 \) is the cutoff radius of the repulsive force that is equal to the distance between neighboring mobile particles in the initial equilibrium distribution. Boundary particles are endowed with a complete set of physical properties, whose contribution is taken into account when approximating the corresponding parameters on the moving particles. However, the boundary particles positions and properties remain unchanged and are not monitored during the simulation.

In the case of describing the inlet and outlet boundary conditions (at least for a supersonic external flow) the introduction of boundary particles is not required. The movable particles leave the computational domain unhindered and disappear when crossing the exit boundary. A new particle with initial parameters determined by the statement of the problem will be created on the inlet boundary instead of the missing one.

The problem of truncating the kernel function arises for the particles located in the immediate vicinity of the boundary. The absence of a sufficient number of neighboring particles near the domain boundaries is compensated by the virtual particles. They are evenly distributed in several layers along the domain boundaries from the outside. The initial locations of the virtual particles are also not changed during the computation. Wherein, the particles of this species participate in the calculation as the nearest neighbors.

The figure 4 shows the initial optimal distribution \([45–49]\) of particles of three above-mentioned types in the solution domain intended for solving the problem of flow past a cylinder in a rectangular channel.

\[
F_{p_{ij}} = \begin{cases}
D \left( \frac{d_0}{|r_j|} \right)^{n_1} \left( \frac{d_0}{|r_j|} \right)^{n_2} \frac{r_y}{|r_j|^2} & \frac{d_0}{|r_j|} \leq 1 \\
0 & \frac{d_0}{|r_j|} > 1
\end{cases}
\]  

(22)

Figure 4. The initial distribution of three sorts of particles in the computational domain.
The meshless method does not impose any restrictions on the degree of deformation of the simulated medium and shape of the integration region due to the high mobility of the freely moving particles and the absence of topological connections between them. The approach is physically reasonable and intuitive. The method does not need to use the computational grid at any of the stages of implementation. The proposed approach guarantees the strict enforcement of the law of conservation of mass, due to the invariance of the mass of each particle. The hybrid technology inherits all the advantages of the Lagrangian and gridless approaches listed above and also uses the strengths of the particle method. Particles are applied not only as interpolation nodes for functions and derivatives, but also act as carriers of medium properties. They accumulate all the necessary information for integrating partial differential equations expressing the conservation laws for the continuous medium.

Moreover, due to a number of features of the simulated systems, it is possible to significantly improve the performance of the method by using efficient nearest neighbor search algorithms and compiling a list of nearest particles, as well as applying high performance computing technologies.

3. Application of the modified particle method to the Sod's shock tube test

The abilities of the modified meshless approach to handle discontinuities and shocks are evaluated on the one-dimensional Sod's shock tube problem [58], which is a particular case of the problem of the decay of an initial discontinuity (Riemann problem). All numerical simulations are performed on a desktop computer with the following hardware: Intel Core i7-3770 CPU3.40 GHz and16 GB RAM. The Fortran 90 language was used to implement the one- and two-dimensional computational models based on meshfree particle method.

Let us consider a long one-dimensional tube, closed at its ends and divided into two equal regions by a thin membrane. Each region is filled with a perfect inviscid gas in two different thermodynamic states $W_{L(0)}$ and $W_{R(0)}$ respectively on the left and right sides of a diaphragm at $x = 0$. The gas is initially at rest ($V_L = V_R = 0$), although the general formulation of the problem of discontinuity decay assumes that velocities are different from zero. The left region is initialized to a higher pressure and density than the right region ($p_L > p_R$, $\rho_L > \rho_R$). The sudden breakdown of the diaphragm at $t = 0$ generates a supersonic flow, which propagates in the low-pressure section. The exact solution of the Riemann problem has a structure consisting of the superposition of elementary waves: shock waves, rarefaction waves and contact discontinuities. In the particular case under consideration the left-going rarefaction fan, right-going shock and a contact discontinuity are implemented (figure 5). As the system evolves, a contact discontinuity moves to the low pressure region (toward the right side), with a shock wave ahead of it, whereas expansion waves propagate to the high pressure region (toward the left side).

![Figure 5](image.png)

**Figure 5.** Statement of the 1D shock tube problem and structure of the exact solution, which contains the shock wave (SW), rarefaction wave (RW) and contact discontinuity (CD).
The region of integration is separated (see figure 5) into four uniform regions with constant parameters (pressure, density, internal energy and velocity): the left (L, I) and right (R, II) regions, which preserve the parameters imposed by the initial conditions, and two intermediate regions, denoted by subscripts III and IV. Across the contact discontinuity pressure and velocity are constant, while the density exhibits a jump from $\rho_{\text{III}}$ to $\rho_{\text{IV}}$. Thus the problem of the exact solution reconstruction reduces to calculating the pressure and velocity values at the contact discontinuity. The iterative procedure for obtaining the exact solution of the Riemann problem by solving the system of nonlinear algebraic equations based on jump relations across discontinuities in perfect gas is described in detail in [59].

The Sod's shock tube problem is defined by the following initial conditions [58]:

$$
\begin{align*}
  x \leq 0: & \quad \rho_I = 1, V_I = 0, p_I = 1, \\
  x > 0: & \quad \rho_{\text{II}} = 0.125, V_{\text{II}} = 0, p_{\text{II}} = 0.1.
\end{align*}
$$

(23)

where $\rho_{\text{I(II)}}, V_{\text{I(II)}}, p_{\text{I(II)}}$ are values of the density, velocity and pressure on the left $x \leq 0$ and right $x > 0$ sides of the membrane. The fluid is initially at rest on either side of the interface, and the density and pressure jumps are chosen so that all three types of flow discontinuity (shock, contact, and rarefaction) develop. The flow variables are nondimensionalized with respect to reference variables on the left high pressure region. The ratio of specific heats $\gamma$ is chosen to be 1.4. The assumptions of absence of viscosity and laminar flow are accepted. The one-dimensional domain of definition of the problem is the closed interval $x \in [0, 1]$, which is divided into high- and low-pressure zones $x \in [-0.5, 0], x \in (0, 0.5]$ by an infinitely thin diaphragm. The investigated process is stimulated with $N=1001$ particles. At zero time, the $N_I = 501$ and $N_{II} = 500$ particles are evenly distributed throughout the high pressure and low pressure regions respectively. The mass of each particle on the left and right sides of the membrane is determined from the following considerations:

$$
\begin{align*}
  m_I^I &= (\rho_I \cdot L_I) / N_I = 9.98004 \cdot 10^{-4}, \\
  m_{II}^I &= (\rho_{\text{II}} \cdot L_{\text{II}}) / N_{\text{II}} = 1.25000 \cdot 10^{-4}.
\end{align*}
$$

(24)

Here $L_{\text{II}} = 0.5$ are the linear extensions of the regions. The time step was set equal to $t = 0.0001$ s. The artificial viscosity (16) is introduced to prevent the appearance of unphysical oscillations [53, 54].

The results of test calculations of one-dimensional shock tube with the considered gridless particle method are shown in figure 6. These data sets presented in the form of density, pressure, velocity and internal energy distributions correspond to the physical time $t = 20$ s (or 2000 time steps). The exact solution of the shock tube problem [59] is placed on the corresponding graph regions for the purpose of comparative analysis. Looking at figure 6, it can be seen that the numerical solution agrees fairly well with the analytical solution. The shock wave is approximately located at $x = 0.35$ and is resolved within several smoothing lengths. The contact discontinuity occupies the interval $0.15 < x < 0.25$, and the rarefaction wave spreads into the region $-0.3 < x < 0$.

For the considered problem there is no need to use of boundary and virtual particles at the ends of the solution domain, since the computation stops before the waves reach the end-walls of the shock tube.

4. Application of the modified meshless approach to the modelling of high-speed flow over a cylinder in a rectangular tube

In order to validate the modified meshless particle method proposed in this paper, the more complicated two-dimensional nonstationary problem of calculating supersonic flow past a circular cylinder placed in a rectangular tube is considered. A circular cylinder is placed in a uniform supersonic flow of an inviscid perfect gas ($\rho_e = 1$ kg/m$^3$ and pressure $p_e = 10^5$ Pa) of velocity $M = 2$. 

13
The cylinder with radius 0.5 is located at the centre of the rectangular channel of length 6 and height 3, through which the high-speed stream flows. The gas medium moves from left to right. The 49 000 mobile particles, as well as 13 000 virtual and boundary particles, are uniformly preallocated in the solution domain (figure 4).

**Figure 6.** The results of testing of the realized meshfree particle method on the 1D shock tube problem by comparison with the exact solution. The physical properties of the $N=1001$ particles, which represent the simulated medium, at time $t=20\ s$.

Figures 7–10 exhibit the snapshots of the flow field at times $t=0.0001, ..., 0.005\ s$ with the pressure, density and longitudinal velocity contours. It is clearly visible from the figures that the shock front moves away from the cylinder surface to the left, upward and downward directions. Once the bow shock wave reaches the tube walls, it is reflected, causing secondary waves. Furthermore the complex flow pattern is resolved fairly well.
These results are also compared with the data obtained using the gas dynamic code developed in Institute for Problems in Mechanics of Russian Academy of Sciences, which is based on the method of splitting into physical processes and unstructured grid finite volume approach [60 – 62] (figure 7).

**Figure 7.** Comparison of computed pressure contours (Pa) for supersonic flow past a cylinder in a rectangular tube at a Mach number of 2 at different times obtained using the present meshless approach (left) and the unstructured grid method [60 – 62], which is second-order accurate in space (right).
Figure 8. Computed pressure contours (Pa) for supersonic flow past a cylinder in a rectangular tube at a Mach number of 2 at different times obtained using the present meshless approach.
Figure 9. Computed density contours ($\text{kg/m}^3$) for supersonic flow past a cylinder in a rectangular tube at a Mach number of 2 at different times obtained using the present meshless approach.
Figure 10. Computed longitudinal velocity contours (m/s) for supersonic flow past a cylinder in a rectangular tube at a Mach number of 2 at different times obtained using the present meshless approach.

5. Conclusion
The meshfree particle method using molecular dynamics techniques for simulating one- and two-dimensional compressible flows was presented in this investigation. One of the main advantages of the present method is its ability to compute 1D and 2D problems (as well as 3D flows in perspective) using the very same code. The detailed description of the approach and its computational implementation was provided to readers. A comparison with the available exact solutions and finite volume reference results for several numerical problems was conducted to test the abilities of the proposed methodology.

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