Numerical modelling of a gas-dust sphere scattering by SPH-IDIC method

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Abstract. The paper is devoted to the first application of the SPH-IDIC method to simulation of three-dimensional dusty gas flow. The expansion of a sphere consisting of gas and monodisperse fine dust into vacuum is considered as a model problem. Computing was carried out using graphic accelerators based on nVidia CUDA technology. The numerical simulations show ability of the method to deal with three-dimensional dynamics. We found that in 3D case the method kept all the advantages previously demonstrated on one-dimensional problems: robustness, efficiency and simplicity in implementation.

1. Introduction

To simulate the dynamics of gas and fine dust mixtures one have to describe intense inter-phase interaction - momentum exchange - between gas and particles. This intense momentum exchange leads to special requirements for numerical methods [1,2]. In particular, new characteristic value arises; it is the relaxation time of phase velocities. Thus, comparing to simulation of pure gas dynamics, adding fine dust to the system affects the time step. In the case of explicit approximation in time, the CFL (Courant-Friedrichs-Lewy) condition serves as a limitation on the time step for pure gas dynamics. However, in dusty gas mixture, if the velocity relaxation time of dust is shorter than the time step, the time step must be reduced to satisfy the stability condition. To get rid of this strict limitation, an implicit approximation of drag terms should be used. Below we will discuss some details of its implementation.

To simulate the dynamics of a multiphase medium, a Smoothed Particle Hydrodynamics (SPH) method is widespread. In this method, the equations of continuous medium dynamics are solved on moving approximation nodes called SPH-particles. In these particles mass, momentum, energy and other parameters of the medium are specified. An approximating function (kernel) is used to calculate the parameters of the medium, and a kernel gradient is used to calculate the spatial derivatives. If function values $f(r_i)$ are known in $N$ SPH particles (interpolation nodes), the function value $f(r)$ at an arbitrary point $r$ of the modeled area can be calculated by basic interpolation formula in SPH method:

$$f(r) = \int f(r')W(r - r')dr',$$

where $W$ is the smoothing kernel, and $h$ is the width of the kernel often called smoothing length.

In this paper we use an approach where gas-dust medium is modeled by sets of particles that correspond to gas as a carrier phase, and dust as a dispersed phase. An inter-phase interaction can be calculated in various ways, in which the general computational complexity and asymptotic properties
of the method will depend on the method of calculating the relative velocities. For the SPH method, three main approaches of spatial velocity interpolation can be distinguished: particle-particle [1], duplicating node [3] and drag in cell [4].

In the particle-particle method [1], neighboring particles of dust phases located at a distance of $2h$ act on each particle of the carrier phase (and vice versa) and the acting is determined by the kernel function. To apply implicit approximation of drag terms in this method we have to know the coordinates and velocities of all surrounding particles in the next time layer, which determines its high complexity. Although so far there are modifications that decrease complexity of this problem [2,5]. In this method, the momentum and angular momentum are preserved in the entire computational domain, but can be violated for an arbitrary volume inside the domain. A short relaxation time of the velocities leads to numerical over-dissipation of the solution, which requires also a decrease in the smoothing length $h$, and an increase in the total number of particles.

The duplicate node method [3] uses the kernel interpolation of the velocity of dust into the point where the gas particle is located. This approach reduces numerical over-dissipation of particle-particle method, but the conservation of both global and local momentum and angular momentum may be lost. For both methods, it is necessary to specify smoothing length according to velocity relaxation time.

The authors proposed the Lagrangian-Euler approach for calculating inter-phase interaction SPH-IDIC [4]. This method allows time step greater than velocity relaxation time and spatial resolution independent of velocity relaxation time. In SPH-IDIC approach, all forces, except drag between phases, are calculated in the usual way for SPH. To compute momentum exchange it uses auxiliary cells in which the average phase characteristics are calculated, and the cell size can be less than the smoothing length.

The paper presents results of three-dimensional simulation of a gas-dust sphere expansion. The three-dimensional implementation of the SPH method requires a large number of particles and the calculation time is greatly increased. Therefore, the IDIC method was adapted for parallel implementation using graphics accelerators based on nVidia CUDA technology.

2. Short description of the model and IDIC method

To simulate the expansion of dusty gas sphere into the vacuum the following assumptions are used. The gas-dust mixture is considered as a medium with a common pressure and zero dust volume fraction. The carrier of the mixture is an inviscid ideal gas. The dispersed phase is considered as pressureless fluid. There is no mass transfer between the gas and the dust, the dispersed phase exchanges momentum with the carrier gas. The particles are monodisperse, i.e. in every local volume, they have only one averaged size.

The description of the whole numerical method based on SPH can be found in [4,6]. Here we will focus only on the way of computing intense momentum exchange. The SPH approximation of motion equations of gas and dust particles is written as follows:

$$\frac{dv^n_g}{dt} = \sum_b m_g \left( \frac{p^n_g}{(\rho^n_g)^2} + \frac{p^n_d}{(\rho^n_d)^2} + \Pi_{ab} \right) \nabla_{ab} W_{ab} - \frac{K^*}{\rho^*_g} (v^{n+1}_g - u^{n+1}_g),$$

$$\frac{dv^n_d}{dt} = \frac{K^*}{\rho^*_d} (v^{n+1}_d - u^{n+1}_d),$$

where $v$, $u$ are the gas and dust velocities, respectively; $\rho_g$, $\rho_d$ are the densities of gas and dust fraction; $m_g$, $m_d$ mass of a gas and dust particle; $\Pi_{ab}$ artificial viscosity. Here we use the cell averages values ($t^*_\text{stop}$ is phase relaxation time and $\rho^*_d$ is density of the dust) and calculated other average in cell values:

$$\varepsilon^* = \frac{m_d L}{m_g N}, \quad K^* = \frac{\rho^*_d}{t^*_\text{stop}}, \quad \rho^*_g = \frac{\rho^*_d}{\varepsilon^*}, \quad v^* = \frac{1}{N} \sum_{i=1}^{N} v_i, \quad u^* = \frac{1}{L} \sum_{j=1}^{L} u_j, \quad A^g_{ij} = \sum_{i=1}^{N} A^g_{ij},$$

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here $L$, $N$ are the numbers of gas and dust particles in the cell, $A_{g,n}^n$ represents all the forces except drag acting on the gas particle. The average velocities on the $n + 1$ layer in each cell are calculated as follows [4]:

$$\frac{\nu_{n+1}^n - \nu_n^g}{\tau} = A_{g,n}^n - \varepsilon_n^g \nu_{n+1}^n - u_{n+1}^n,$$

$$\frac{u_{n+1}^n - u_n^g}{\tau} = \frac{\nu_{n+1}^n - \nu_n^g}{\tau}$$

Velocities of each particle at new time layer are calculated:

$$\left(\frac{1}{\tau} + \frac{\varepsilon_n^g}{t_s^n}\right) \nu_{n+1}^n = \frac{\nu_n^g}{\tau} + \frac{\varepsilon_n^g}{t_s^n} u_{n+1}^n + A_{a,n}^n,$$

$$\left(\frac{1}{\tau} + \frac{\varepsilon_n^g}{t_s^n}\right) u_{n+1}^n = \frac{u_n^g}{\tau} + \frac{1}{t_s^n} \nu_{n+1}^n$$

The equations are supplemented by the equation of state of the gas, in our case the gas was assumed to be ideal:

$$P_{n+1}^a = \rho_{g,a}^{n+1} \varepsilon_{g,a}^{n+1} (\gamma - 1)$$

and energy equation:

$$\frac{d\rho_{a}^n}{dt} = m_g \rho_{a}^n \sum_b (\nu_{n}^g - \nu_{n}^a) V_{ab} W_{ab} + m_g \frac{\Pi_{ab} (\nu_{n}^a - \nu_{n}^b)}{2}$$

At the beginning of the calculation, we divide the entire computational domain into disjoint volumes so that the union of these volumes coincides with the entire domain. This step is performed on the CPU, since the volumes do not change with time and it is enough to perform this once before the main calculation cycle.

Supposing that the coordinates, velocities, densities of gas and dust particles, as well as the internal energy of gas particles are known on the time layer $n$, we will find these quantities on the layer $n + 1$.

- **Calculation of acceleration** ($A_{g,a}^n$) from all forces except friction that act on particles on the layer $n$. This step coincides with the corresponding step in the classical SPH method and is implemented on the GPU. The acceleration calculation procedures works parallel an array of particles, and they themselves are called in a cycle along the neighboring particles.

- **Calculation of the average values for each cell of the $n$ layer.** This step requires a single pass through all particles and its parallel implementation creates problems with memory access collisions when accumulating the sums over the cells, therefore this step is implemented on the CPU.

- **Calculation of average velocities in cells on the layer $n + 1$ is performed on the GPU in a parallel manner.**

- **Velocity calculation on the $n + 1$ layer is implemented on the GPU in parallel for particles of each phase.** Calculations for each phase are performed sequentially. That is, first, gas particles are processed in parallel, and then dust particles are also processed in parallel.

- **The calculations of the new coordinates, densities, pressure and energy do not differ from the classical SPH method and are performed on the GPU by the corresponding parallel procedures.**

This implementation showed good results both in calculation time and in the total number of particles. Test calculations showed that it is possible to carry out calculations with several million particles of each phase in an acceptable time.

### 3. Expansion of a gas-dust sphere

To run a simulation we suppose that a gas-dust mixture rests at the initial moment and occupies a spherical volume of radius 1.0 centered at the origin of coordinate system. The initial parameters of the medium were set as follows: gas density $\rho_g = 1.0$, dust density $\rho_d = 0.5$, energy in the gas $e = 2.5$, pressure $p = 1.0$. The relaxation time for dust was chosen small, at the initial moment $t_{stop} \approx 8.45 \cdot 10^{-4}$, and later, despite a local increase in relaxation time, it remained small as compared to the calculation time. The initial relaxation time was significantly less than the time step $\tau = 0.005$. 

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Initially, the SPH particles were arranged uniformly along the Cartesian grid. We used \( \approx 247000 \) particles for every phase, the smoothing length was \( h = 0.1 \), and the drag cell size in the IDIC method was \( 0.5h \).

![Figure 1](image1.png)

**Figure 1.** Distribution of gas and dust SPH particles in space and in projection onto the XYZ plane at \( t = 0.2 \).

A general view of the gas and dust sphere at time \( t = 0.2 \) is shown in the left panel of Figure 1. We can see that during the expansion of the sphere the central symmetry is preserved. In the right panel of Figure 1 a projection of model particles on the plane perpendicular to \( z \) axis is shown. We can see the rarefaction wave propagating from the free surface. Moreover, some separated particles outside the sphere are clearly visible. This particle emission is associated with initial distribution of particles in Cartesian grid nodes that does not take into account central symmetry of the simulated configuration.

![Figure 2](image2.png)

**Figure 2.** Dust and gas density profiles, pressure in the medium and gas energy at \( t = 0.2 \)

Left panel of Figure 2 shows the distribution of gas and dust densities over the radius near the boundary at time \( t = 0.2 \). As it is noted above, by this time a rarefaction wave was formed. It should be noted that there are "not enough" neighbors for particles located at a distance of \( 2h \) from the free
surface. Thus, we see a density drop near the free surface. This numerical artefact also affects the gas pressure and inner energy (see right panel of Figure 2), velocity values of gas and dust (see left panel of Figure 3) where pronounced perturbations are seen near the boundary of the configuration. Moreover, from the left panel of Figure 3 it follows that the computed velocity of the dust is noisier than the velocity of the gas.

On the other hand, inside the sphere the distribution of gas and dust parameters is in good agreement with analytical expectation. In particular, the gas pressure repeats the density profile. In rarefaction wave, the gas velocity depends linearly on radius. The left panel of Figure 3 shows that the dust moves synchronously with the gas, since its relaxation time is much shorter than the simulation time (see right panel of Figure 3). As a result of synchronous dynamics, the dust turns out to be "frozen" into the gas. This is clearly visible in the left panel of Figure 2, where the features of the wave profiles at densities almost coincide. Moreover, the right panel of Figure 3 confirms that SPH-IDIC method allows simulation with the time step bigger than the velocity relaxation time.

![Figure 3. Distribution of the magnitude of phase velocities and the value of the local relaxation time in particles at t = 0.2.](image)

**Conclusions**

The paper is devoted to the first application of SPH-IDIC method to simulation of three-dimensional dusty gas flow. We simulated the expansion of a sphere into the vacuum. The sphere consisted of ideal gas and monodisperse fine dust. The dust had a small velocity relaxation time, the concentration of dust was high, and the mutual momentum exchange was taken into account.

The first simulations were done with rough numerical resolution: we used only 247000 particles for each phase and time step bigger than velocity relaxation time. We found that SPH-IDIC method is robust and able to capture the main features of the flow even with rough numerical resolution.

To implement the IDIC method of drag computing we used Cartesian grid, which was inconsistent with the spherical symmetry of the dynamics. However, we found that during the expansion the spherical symmetry of the configuration is preserved with acceptable accuracy.

As next steps, we plan (1) to obtain the quantitative estimation of asymptotic properties of the SPH-IDIC method on three-dimensional problems with known reference solution, (2) to implement the SPH-IDIC on distributed memory machines, and (3) to perform multidimensional simulations of gas with polidisperse dust.
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