Numerical modelling of levitating particles in air

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Abstract. A numerical model for the particles levitation in an ultrasonic field is developed on the basis of the finite difference time domain method. The force effect of the ultrasonic field on the particles is calculated via gradient of the Gor’kov potential, also the friction force in gases for spherical particles is taken into account. With the help of the OpenCL technology, a parallel computation of the trajectories of a set of particles is implemented.

1. Introduction
The control of particles in the ultrasound field has recently received considerable attention. The technology of acoustic levitation of particles in the air has prospects for use as contactless tweezers for manipulating small objects. Such methods will be used in 3D printing, medicines manufacturing, for the manufacture of complex chemical composites. In the work of Gor’kov, an expression for radial pressure on a small spherical particle is given [1]. In work [2] is presented a technology of manipulation by levitating particles using phased arrays of ultrasonic sources. Acoustic field can cause such effects as attraction and repulsion [3]. Acoustic effects on particles attract the attention of researchers [4–7]. Numerical simulation of acoustic levitation is important part preliminary to experimental research. In [8] has been proposed a single frequency numerical method to calculate potential for acoustic radiation force on the basis of matrix representation. We propose a numerical model of levitating particles in gases optimized for parallel computing on the basis of finite difference time domain method. The simulated ultrasonic field is represented as a set of harmonic waves and stored in memory as a set of complex coefficients.

2. Mathematical model
To predict the behavior of particles in the ultrasonic field, it is necessary to conduct a numerical simulation of the effect of the ultrasonic field on the particles.

The calculation of the force acting on a particle in an ultrasonic field can be accomplished using the Gor’kov formula [1]:

\[ \mathbf{F} = -\nabla U, \]

where \( U = 2\pi R^3 \rho \left( \frac{p^2}{3\rho c^2} f_1 - \frac{v^2}{2} f_2 \right) \) – Gor’kov potential, \( f_1 = 1 - \frac{c^2}{c_0^2 \rho_0}, \)

\( f_2 = 2 \frac{\rho_0 - \rho}{2\rho_0 + \rho}, \)

\( \rho \) – density environment (air), \( \rho_0 \) – particle density, \( p \) – acoustic pressure, \( v \) – acoustic velocity, \( \overline{p^2} \) – average of field pressure square, \( \overline{v^2} \) – average of field velocity square.
The particle trajectory is modeled based on the equations of motion: \( \mathbf{r}(t + \Delta t) = \mathbf{r}(t) + \mathbf{v}(t)\Delta t + \mathbf{a}\Delta t^2 / 2 \) – coordinates of the particles in the next time, \( \mathbf{v}(t + \Delta t) = \mathbf{v}(t) + \mathbf{a}\Delta t \) – particle velocity, \( \mathbf{a} = \left( \mathbf{F} + \mathbf{F}_f + \mathbf{F}_{fr} \right)/m \) – particle acceleration, \( m \) – particle mass, \( \mathbf{F}_f \) – friction force, \( \mathbf{F}_{fr} \) – gravity force.

The speed potential of wave field is defined as a set of harmonic waves:
\[
\Phi(\mathbf{r}, t) = \sum_n A_n(\mathbf{r})\cos(\omega_n t + \varphi_n(\mathbf{r})),
\]
where \( \omega_n \) – cyclic frequency of nth harmonic, \( A_n(\mathbf{r}) \) – magnitude of wave field at point \( \mathbf{r} \), \( \varphi_n(\mathbf{r}) \) – phase of wave field at point \( \mathbf{r} \). For each wave defined magnitude \( A_n(\mathbf{r}) \) and phase \( \varphi_n(\mathbf{r}) \) in different points of media by solving Helmholtz equation for frequency \( \omega_n \). To minimize computational efforts for field calculation we propose to calculate field pressure and velocity only at points of particles location. Pressure of acoustic field is calculated via speed potential by following operation:
\[
p(\mathbf{r}, t) = -\rho \frac{\partial \Phi(\mathbf{r}, t)}{\partial t} = \rho \sum_n A_n(\mathbf{r})\omega_n \sin(\omega_n t + \varphi_n(\mathbf{r})).
\]
The speed is defined as: \( \mathbf{v} = \nabla \Phi \), numerically we calculated it by expression:
\[
\mathbf{v}(\mathbf{r}, t) = \begin{pmatrix}
x_0 \frac{\Phi(\mathbf{r} + \mathbf{x}_0\Delta x, t) - \Phi(\mathbf{r} - \mathbf{x}_0\Delta x, t)}{2\Delta x} \\
y_0 \frac{\Phi(\mathbf{r} + \mathbf{y}_0\Delta y, t) - \Phi(\mathbf{r} - \mathbf{y}_0\Delta y, t)}{2\Delta y} \\
z_0 \frac{\Phi(\mathbf{r} + \mathbf{z}_0\Delta z, t) - \Phi(\mathbf{r} - \mathbf{z}_0\Delta z, t)}{2\Delta z}
\end{pmatrix},
\]
where \( \mathbf{x}_0 = (1,0,0), \mathbf{y}_0 = (0,1,0), \mathbf{z}_0 = (1,0,0) \) – orthogonal unit vectors, \( \Delta x, \Delta y, \Delta z \) – spatial steps of field calculation for \( x, y \) and \( z \) axis respectively. To calculate force acting on the particle via formula (1) it is required to evaluate gradient operator that requires definition of field in 6 points for numerical computation of symmetrical spatial derivative. Overall, to find acoustic force acting on the particle it is required to calculate \( \Phi(\mathbf{r}, t) \) at 19 different points, where \( \mathbf{r} \) – is the coordinates of the particle.

We used the OpenCL technology for the software implementation of the algorithm for calculating the trajectory of levitating particles in the ultrasonic field. This technology allows you to perform parallel computing on the set of cores of the graphics card processor. Consider the possibility of launching M parallel threads; then, to calculate the trajectories of N particles, it will be necessary to calculate the positions of N/M different particles in each thread. Arrays containing data on the coordinates and velocities of particles are stored in the graphics card’s memory to reduce data exchange with the central processor. The ultrasound field is defined as three-dimensional arrays of complex numbers for various frequencies, which are loaded into the memory of a video card before the simulation of particle motion begins.

3. Numerical modeling
For numerical test we propose to compute particles dynamics in wave field of special configuration (Figure 1). We consider that source field is generated by planar phased array at frequency 22 kHz and allows forming the focused wave field of the letter “R” shape at distance 20 cm.

Under the focusing plane we placed planar reflector to create standing wave. Particles should levitate at a quarter of a wavelength above the reflector and concentrate around local maxima of field.

Software was developed based on the OpenCL parallel programming technology for simultaneous calculation of the trajectory of many particles in an ultrasonic field. Considered source field is shown on Figure 2a, and resulting focused field above the reflector is shown on Figure 2b. The result of particle trajectories modeling show on Figure 3.
Figure 1. Considered numerical test of particle levitation.

Figure 2. Speed potential field of plane phased array source: a – at the source plane; b – at focus plane.

Figure 3. The initial distribution of particles (a) and after 2 s (b) in an ultrasonic field with a frequency of 22 kHz and an amplitude of 1.2 kPa.

Modeling of levitation of plastic particles with density 1050 kg/m$^3$ and diameter of 100 to 1000 µm
was carried out in the considered ultrasonic field with a frequency of 22 kHz in air with a speed of sound of 343 m/s. On the vertical axis, the field has a maximum corresponds to focusing distance that equal to 20 cm, which should provide levitation in the field of gravity. The developed program made it possible to calculate the positions of 2048 particles with a random initial coordinate distribution (Figure 3a) and to obtain the position of the particles after 2 s (Figure 3b).

We can observe concentration of particles into letter “R” shape. Particles tend to local field maxima, which does not allow the formation of images with homogeneous regions. From here we can conclude that a single array of emitters is not enough to form an arbitrary image. The behavior of the particles does not contradict to theoretical expectations.

4. Conclusion
A numerical model of particle levitation in an acoustic field has been developed suitable for parallel computation. We proposed to represent an ultrasonic field as a set of harmonic oscillations in the whole modeling space, and further calculate the time dependence of the field only at the points where the particles are located. This approach saves the memory required for storing a three-dimensional field at different points in time. The calculation of the acoustic force acting on the particles requires the determination of the field at 19 neighboring points. The field is found by summing the harmonic components of waves, taking into account their amplitudes and phases. The performed simulation has shown results that are consistent with theoretical expectations.

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