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Guskova Mariia

Drop motion simulation in confined geometry

PhD Dissertation Summary
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Doctor of Philosophy in Applied Mathematics

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Doctor of physical and mathematical sciences,
professor
Shchur Lev

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Research relevance

Microfluidics is a branch of fluid dynamics that studies fluid flow in small volumes. Microfluidic devices often solve problems in medicine and microbiology: sorting blood cells by size, ordering cells in the flow, detecting pathogens, performing operations of adding tags to cells for their further sequencing and others.

Particles or droplets of another fluid may form an ordered structure in the flow in which the particles are approximately equally spaced apart. Such structures are called "floating" crystals because of their periodicity property. Crystals may appear due to external forces (electric or magnetic field) or due to hydrodynamic interaction of particles with each other. Based on the type of particles, crystals are divided into droplet crystals, inertial particle crystals, viscoelastic particle crystals and compartmentalized [Del Giudice et al., 2021] crystals. Microfluidic crystals are interesting because of fundamental problems and because of their practical applications in synthesizing colloidal structures, performing digital polymerase chain reaction (PCR) and single cell analysis (a type of biological experiments where one needs to qualitatively and quantitatively characterize the RNA molecules found).

Droplet crystals are studied in physical experiments[Beatus et al., 2006, Schiller et al., 2015] and by computer simulation [Uspal and Doyle, 2012, Schaaf and Stark, 2020, Janssen et al., 2012]. The authors of [Beatus et al., 2006] paper describe an experiment where transverse and longitudinal oscillations are found in a one-dimensional crystal of water droplets moving in oil. These oscillations are similar to phonons in solids. The emergence of the spectrum is explained by the dipole-dipole interaction of the microparticles due to the large velocity difference between the microparticles and the surrounding flow. It seems important to investigate the question: is this mechanism the only explanation of the phonon spectrum appearance?

In this work, microfluidic crystals of droplets and particles without the influence of external forces are considered. Computer simulation is carried out using the lattice Boltzmann method (LBM) [Krüger et al., 2013].

Problem statement

The aim of the work is to investigate the mechanisms of the phonon spectrum emergence in a crystal of droplets. In the two-dimensional channel at small Reynolds numbers, the particles move approximately with the flow velocity and because of this there is no significant dipole-dipole interaction between the droplets, which allows us to check the influence of other phenomena, such as hydrodynamic interaction with the walls.

The study is carried out using computer simulation: numerical integration of ordinary differential equations, simulation of the flow and other liquid droplets placed in it using a three-dimensional model of the LBM and the Shan-Chen model, and two-dimensional simulation of the flow and solid particles placed in it using the LBM and the immersed boundary method.

The main tasks of the work are:

1. To investigate the effect of droplet oscillations on the motion of a chain of droplets.

2. To test whether dipole-dipole interaction can actually generate the spectrum observed in experiments.

3. To obtain the phonon spectrum in the crystal of particles without significant dipole-dipole interaction and to study the reasons for its occurrence. To investigate the influence of the equilibrium position of the particle chain on the phonon spectrum.

Additional tasks:

1. Investigate the effect of initial conditions (symmetry, angular velocity, and linear velocity) on the motion of a single particle in a confined space.

2. Evaluation of the accuracy of LBM boundary conditions in the frame of POiseuille flow simulation.

3. Code validation on the Segre-Silberberg effect and computation of equilibrium positions for particle chains.

Current state of the research topic

Authors of the [Beatus et al., 2012] present the results of a series of experiments on microfluidic crystals. The crystal consists of water droplets that move in oil. Because of the friction of the droplets against the upper and lower walls of the channel, the velocity of the droplets is about 5 times less than the velocity of the main flow. Because of this significant difference in velocity, there is a dipole-dipole interaction between the droplets. Droplets in a crystal are not strictly located at equal distances and on the central axis, but with some random displacement caused by the channel imperfection (wall flatness), asymmetry of the droplet generator. In a one-dimensional chain of droplets, longitudinal and transverse oscillations appear, the spectrum of which is similar to the phonon spectrum. The authors [Beatus et al., 2012] explain the appearance of the phonon spectrum exclusively by the dipole-dipole interaction. To check this, they integrate the ordinary differential equations for dipoles and the numerically obtained spectrum is similar to the real one. Similarly, in [Liu et al., 2012] the results of numerical integration of the droplet equations of motion obtained in [Beatus et al., 2006] are shown. Unlike the oscillation spectra of the physical experiment, there is no straight line in the spectrum because it arises due to defects in the channel.

The motion of particles in the channel at low Reynolds numbers is influenced by the proximity of the walls (that slow down the particles), by the viscosity of the fluid, by the velocity of the particles relative to the flow velocity, and by the rotation of the particles. In [Segre and Silberberg, 1961] it is shown that particles in a cylindrical Poiseuille flow concentrate in a ring at some distance from the walls and the central axis. In another [Oliver, 1962], it is shown that if there is no rotation, the particles converge to the central axis. The [Saffman, 1965] derives a formula for the lift force that acts on a particle, $81.2Va^2\kappa^{1/2}/\nu^{1/2} + o(\nu^{-1/2})$, where $V-$ flow velocity, $a-$ particle radius, $\kappa-$ flow velocity gradient, $\nu-$ kinematic viscosity. There are limitations of analytical work: very small Reynolds numbers [Saffman, 1965, Rubinow and Keller, 1961] or moderate Reynolds numbers [Asmolov et al., 2018], small value of the ratio of particle diameter to channel diameter [Saffman, 1965, Rubinow and Keller, 1961], inability to evaluate the effects of droplet oscillations and reflected waves from the channel walls. In computer simulation works, on the contrary, it is more difficult to simulate small Reynolds numbers because of the necessity to use very low velocity or high viscosity. In works [Yang et al., 2005, Esipov et al., 2020] the influence of Reynolds number on the particle equilibrium position is investigated and the increase of the Reynolds number leads to the fact the shift of equilibrium position to the channel wall. Another parameter of the problem is the ratio of particle diameter to channel diameter γ. The increase of the γ leads to shift of the equilibrium position of particles to the center of the channel.

For the simulation of inertial microfluidics, methods based on the solution of the Navier-Stokes equations or LBM [Bazaz et al., 2020] methods are used. Inertial microfluidics refers to the migration of randomly distributed particles to some equilibrium positions within a microchannel as a function of particle size. Methods based on solving the Navier-Stokes equations have difficulty in determining the interface between the droplet or particle and the flow, also these methods are time consuming. LBM has an advantage because of the relative ease of parallelization of the algorithm and the multitude of models for different physics, including the modeling of droplets of one fluid inside another.

Methodology

The study relies on computer simulation results. The LBM and the Shan-Chen model for multicomponent liquids[Shan and Chen, 1993] are used to simulate liquid droplets placed in another liquid. Rayleigh's analytical formula for the oscillation frequency of a [Rayleigh, 1879] droplet is checked to evaluate the simulation accuracy. The immersed boundary method [Inamuro, 2012] coupked with LBM is used to compute moving solid particles in the flow. To evaluate the validity of these methods, the simulation-derived oscillation spectra of the microfluidic crystal were compared with the results of a physical experiment[Beatus et al., 2006].

General findings of the study

Influence of drop oscillations on a chain of drops

In a one-dimensional droplet chain, instabilities sometimes occur that lead to crystal collapse [Beatus et al., 2012]. In the thesis work, simulations of the droplet oscillations were performed to evaluate the effect on neighboring droplets. It turned out that droplet oscillations can affect the stability of the droplet chain if the velocity of the injected droplets v_d multiplied by the droplet spacing a is close to the lowest Rayleigh frequency, i.e., $v_d\, a \approx \omega_2/2\pi$. The effect would lead to a deformation of the droplet, a change in the distance between the droplets, and a change in the axial symmetry of the chain. Perhaps it is this resonance that can explain the disorder in the experiments [Beatus et al., 2012].

The multicomponent Shan-Chen [Shan and Chen, 1993] multicomponent fluid model for two immiscible liquids is used. In a rectangular parallelepiped, where all faces are walls, three drops of equal volume were placed on the central longest axis. The drops and the surrounding medium have the same viscosities and densities. The central drop at the initial moment of time is stretched along the axis Z, thus excites ω_2 frequency. Once the simulation starts, the central droplet starts to oscillate and although the oscillations are damped due to viscosity, the sound waves start to move neighboring droplets to the walls and deform them. The period of natural oscillations of the drop is smaller than the period of phonon waves in the chain, so the change of the shape cannot be the cause of the phonon spectrum in the chain.

Chain of vortices pairs

To further verify the dipole interaction as a cause for the phonon spectrum, a chain consisting of pairs of point vortices with opposite sign circulations was realized in the droplet crystal. The spectra for the emerged oscillations in the chain are qualitatively similar to the spectra in the [Beatus et al., 2006].

We consider a system of $2 \cdot N$ vortices with circulations $\kappa_i (i = 1, \ldots, N)$, $N = 32$ – the number of vortex pairs, i.e., dipoles. Coordinates of vortices $x_i, y_i (i = 1, \ldots, N)$. The Hamiltonian of such a system is defined by the expression [Manakov and Shchur, 1983]:

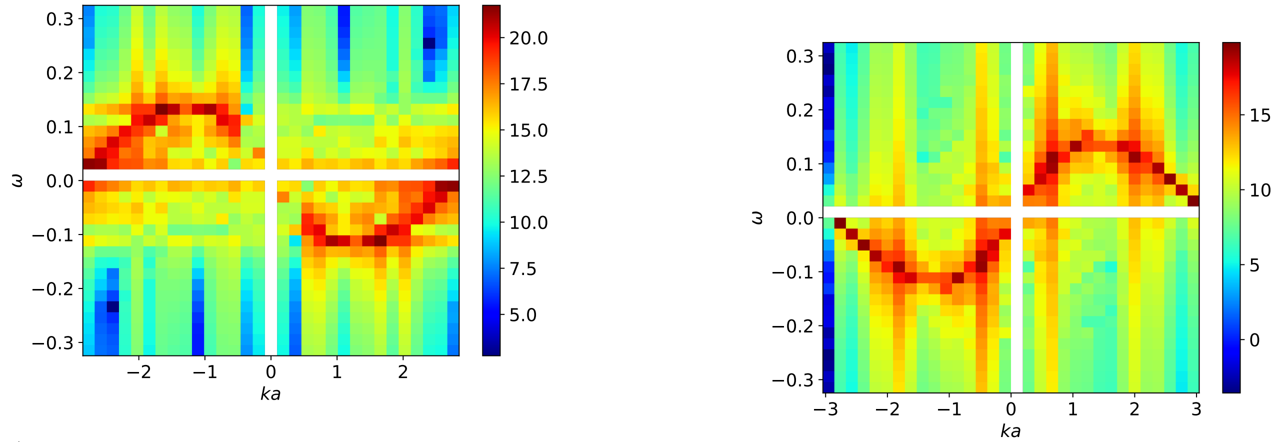
$$H = \frac{1}{2} \sum_{i<j} \kappa_i \kappa_j \ln[(x_i - x_j)^2 + (y_i - y_j)^2].$$

Then the equations of motion are written in the following form:

$$\dot{x}_i = \{x_i, H\}, \dot{y}_i = \{y_i, H\}, \tag{1}$$

where Poisson brackets are defined as $\{A, B\} = \sum \kappa_i^{-1} (\frac{\partial A}{\partial x_i} \frac{\partial B}{\partial y_i} - \frac{\partial A}{\partial y_i} \frac{\partial B}{\partial x_i})$.

Periodic boundary conditions along the X-axis are used. The vortices in a pair with index i are shifted at each integration step by the same vector $(\dot{x}_i, \dot{y}_i) = (0.5(\dot{x}_i^0 + \dot{x}_i^1), 0.5(\dot{y}_i^0 + \dot{y}_i^1))$, which is the average displacement for the vortices in this pair.



(a) Spectrum of the longitudinal oscillations

(b) Spectrum of the transversal oscillations

Figure 1: Spectra of vortices pairs oscillations

Figure 1 shows the oscillation spectra for ξ, y coordinates, where ξ is the X distance between neighboring pairs of vortices and y is the $y-$coordinate of the upper of the vortices in the dipole. The spectra were obtained using the two-dimensional fast Fourier transform in space and time.

Phonon spectrum

In this work, a phonon spectrum for a crystal made of rigid particles that moves approximately at the flow velocity was obtained using IB-LBM simulation. Since the velocities are close, there is no significant dipole interaction between the particles and the appearance of oscillations in the crystal is explained by the influence of waves reflected from the walls.

Using the immersed boundary method together with LBM to calculate the [Inamuro, 2012] flow, the motion of rigid round particles in Poiseuille flow was simulated. A 2D problem was considered. In the paper [Beatus et al., 2012] a quasi-dimensional problem is considered: the height of the channel is much smaller than its length and width. Because of friction against the walls the droplets move slower than the main flow. Also, in contrast to the physical experiment, the density of the particle is the same as the density of the surrounding liquid.

The computational domain is a long channel, at the top and bottom of the channel the boundary conditions are no-slip – walls, along the axis X periodic boundary conditions. At an initial time, particles of radius $R = 10$ are placed on the central axis of the channel of width $W = 40$ with distance between particle centers $a = 4R$. A small random perturbation is added to the particle coordinates. The Reynolds number $Re = 0.5$.

For such channel parameters, the equilibrium position of the particles is on the central axis, the particles try to converge to this position, but hydrodynamic interaction with the others leads to oscillations across the axis. The transverse oscillations are more pronounced than the longitudinal oscillations and their spectrum is similar to the results of the [Beatus et al., 2012] experiment. Longitudinal oscillations in this setting have a longer period than transverse oscillations and require a long simulation time to obtain a high-quality spectrum, which is complicated by the fact that periodic boundary conditions lead to the particles synchronization with each other and the spectrum of their oscillations becomes linear.

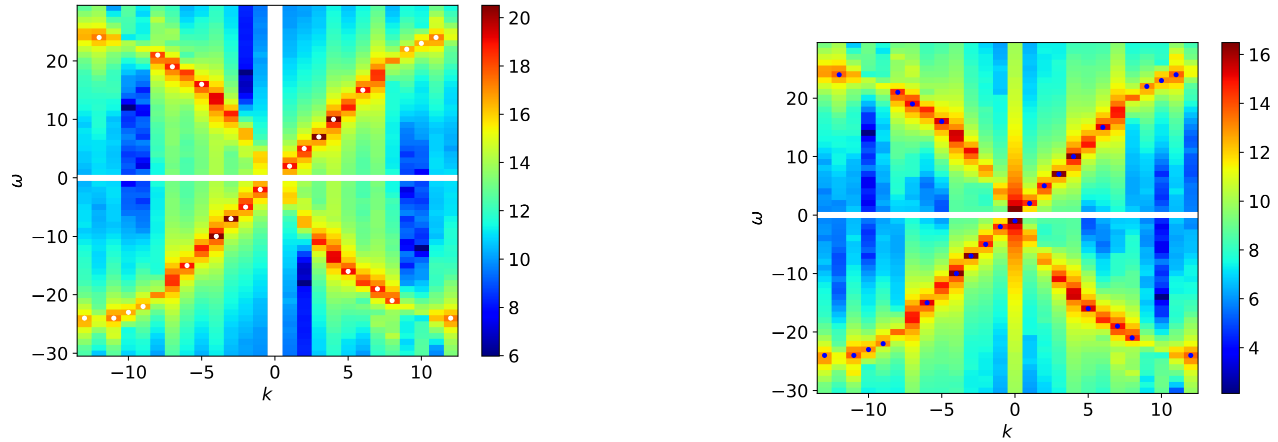
Phonon spectrum for different equilibrium positions

The longitudinal and transverse oscillations spectra were obtained for a crystal placed close to the wall.

For the wide channels, the equilibrium position on the central axis is unstable and the position on some axis between the center and the wall – stable. For example, for channel width $W = 80$ and particle radius $R = 10$, such an axis is $y/W \approx 0.748$ and symmetric to it $y/W \approx 0.252$.

As the chain is shifted to the wall and the ratio of the particle diameter to the channel width is reduced longitudinal oscillations appear in the crystal due to asymmetric hydrodynamic interaction with the wall (Fig.2). It is surprising that even and odd particles move out of phase, and its spectrum looks like spectrum of a chain with atoms of alternating masses. The spectrum for even (and odd) particles has an optical branch (Fig.3).

The oscillation spectrum in a chain with alternating particles does not depend on the particle density. When the radius is changed, the chain breaks up into two chains, but they continue to oscillate together, and again there is an optical branch in the spectrum. The frequency of longitudinal oscillations decreases with increasing distance between particles, but even when the distance is doubled, the unit cell consists of two particles.



(a) Spectrum of the longitudinal oscillations

(b) Spectrum of the transversal oscillations

Figure 2: Spectra of the oscillations in the crystal placed at $y/W = 0.748$ axis in the channel of width $W = 80$.

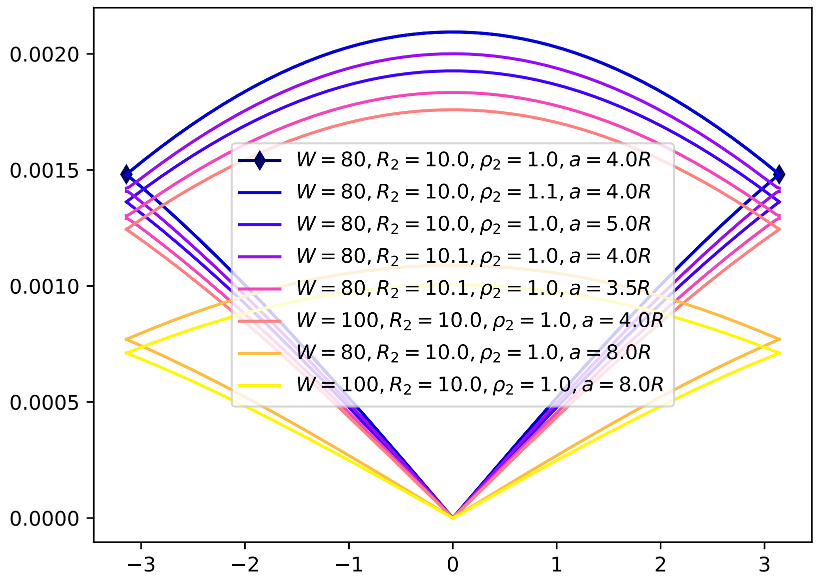


Figure 3: The dispersion relations for the longitudinal waves

Computational tools

For the simulation of oscillating soft drop the C++/MPI library Palabos [Latt et al., 2020] library was used. A bug in the generation of oscillating flow "https://gitlab.com/unigespc/palabos/-/issues/14" was fixed during this work, and corrections were applied to the library. To simulate the chain of particles in Poiseuille flow, a code in Python 3.8 was developed with the use of numpy and numba.The code is available in the repository https://github.com/msguskova/lbm_chain_of_particles [Guskova, 2023].

Thesis statements

1. The characteristic time of stability of the oscillating drop has been estimated using LBM simulation. The oscillations dampen in a time shorter than the wave's period in the chain of particles, and therefore they cannot have a significant influence.

2. Influence of the drop's natural oscillations on neighboring drops has been investigated and characteristic time till nearby drops start to move is evaluated. Mutual influence of shape oscillations does not notably impact on collective oscillations.

3. The mechanisms of the emergence of particles oscillations in Poiseuille flow have been investigated. The oscillations are caused by interaction with the channel's walls. For the first time optical branch in spectrum has been demonstrated in microfluidic crystal. Such spectrum appears if the equilibrium position of the particle chain not on the symmetry axis.

Scientific novelty

1. The hypothesis that the natural oscillations of droplets can cause oscillations in a chain of droplets has been tested.

2. It was shown that the phonon spectrum in a microfluidic crystal can be caused by hydrodynamic interaction with the channel walls. Earlier in the [Beatus et al., 2006] paper, the dipole-drop interaction was pointed out as the cause of oscillations. In our setup, the velocity of particles relative to the main flow is small (less than 5%), so there is no appreciable dipole-dipole interaction.

3. An optical branch in the spectrum of longitudinal and transverse oscillations in a crystal located not on the symmetry axis is demonstrated.

Approbation of the results

1. "Use of the $\sqrt{2/3}$ sound speed model in the lattice Boltzmann method for the example of particle motion in Poiseuille flow", E.V. Armensky Interuniversity Scientific and Technical Conference of Students, Postgraduates and Young Specialists, 27.02-7.03.2023, Moscow, Russia.

2. "Wave spectrum of the flowing drops", Supercomputer Days in Russia, September 27-28 2021, Moscow, Russia

3. "Drop chain simulation with Lattice Boltzmann method", 29th International Conference on Discrete Simulation of Fluid Dynamics, September 13-17 2021, Viterbo, Italy.

4. "LBM simulation of the chain of three drops", Conference on Computer Simulation in Physics and beyond, October 12-16, 2020, Moscow, Russia.

Articles

All publications are indexed in the Scopus international citation system.

1. Guskova M. et al. Simulation of the Particle Dynamics in the Two-Dimensional Poiseuille Flow with Low Reynolds Number //Lobachevskii Journal of Mathematics. 2022. Vol. 43. No. 2. P. 381-385.

2. Guskova M., Shchur V., Shchur L. Simulation of drop oscillation using the lattice Boltzmann method //Lobachevskii Journal of Mathematics. 2020. Vol. 41. No. 6. P. 992-995.

3. Guskova M., Shchur L. Immersed boundary simulation of drop stability //Journal of Physics: Conference Series. – IOP Publishing, 2021. Vol. 1740. No. 1. P. 012026.

4. Guskova M., Shchur L. Wave Spectrum of Flowing Drops //Russian Supercomputing Days. – Cham : Springer International Publishing, 2021. P. 283-294.

5. Shchur L., Guskova M. Drop Oscillation Modeling //Russian Supercomputing Days. – Cham : Springer International Publishing, 2020. P. 198-206.

Personal contribution of the author to the development of the problem

The ideas proposed in the thesis were put forward by the applicant together with her supervisor. The author independently developed the code, conducted computational experiments, and processed the results. The author personally reported the results of the work at the mentioned conferences and wrote the main part of the paper 4.

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