Internship report: Theory and simulation of the acoustic radiation force on a suspended microparticle

Nicolas Vauchel

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This report aims to present the study of the influence of different properties on the radiation force in a microfluidic system.

I have been welcommed as an intern by the Theoretical Microfluidics group at Danmarks Tekniske Universitet(DTU), Technical University of Denmark.

In all the report, vectors will be underlined and second-order tensors will be double underlined.

Contents

1 Acknowlegments

I would like to aknowledge Professor Henrik Bruus, my internship supervisor, who has always been available for me.

I would like to thank the PhD studends Mikkel W.H. Ley, Jacob Søberg Bach, Nils Refstrup Skov and postdoctoral fellow Wei Qiu for all the help they brought me.

Finally, I would like to aknowledge DTU, Centrale Lille and the University of Lille 1 for giving me the chance to have this experience.

2 Presentation of the university and of the team

2.1 Presentation of the university

DTU main campus is located in Kongens Lyngby, a town in the North of Copenhagen. It was created in 1829 and was first located in the heart of the Denmark capital city. With a growing number of students, new buildings were created and the university finally set up in Lyngby in the early 1960's.

Concerning statitics about DTU: according to the DTU website, the total employed staff was of 6,000 people and there were 11,000 enroled students in 2016. To give a factor of the activity of the university, researchers made more than 5700 publications during the same year.

DTU's research activity is segregated in 22 departments wich cover a lots of fields in Physics, Managment, Chemistry, Engineering, Mathematics, Biology, Medicine, and Computer sciences. The group I joined is a part of the department of Physics (http://www.fysik.dtu.dk/english).

Every departments are divided into sections, composed themself of the research groups. The department of Physics is composed of 6 different sections: "Computational Atomic-scale Materials Design", "Nanoparticle and Surface Science", "Biophysics and Fluids", "Material Physics and Large Scale Facilities", "Plasma Physics and Fusion Energy" and "Quantum Physics and IT". The Theoretical Microfluidics group is a part of the "Biophysics and Fluids" section. This section aims to study Biophysics and Fluid Dynamic over a wide range of scales, from big structures conducted by turbulences to microscales.

2.2 Presentation of the research group

The Theoretical Microfluidics Group studies Fluid Mechanics at the micrometer and nanometer scales. Its principal objectives are to create theoretical models and numerical simulations of actual microdevices. The group also collaborates with experimental teams.

The team is composed of PhD students and postdoctoral fellows and is led by Prof. Bruus. The Ph.D. students I worked with were: Mikkel W.H. Ley, Jacob Søberg Bach and Nils Refstrup Skov. I also worked with postdoctoral fellow Wei Qiu. I was very well integrated in this team. I shared an office with Mikkel, and a computer was lent to me. Every week, I met face to face with my supervisor about one hour. Every Tuesday, we met for group meeting, where each member talked about the status of his work and coming plans. That permitted to bring some help and some ideas.

There was a very good atmosphere within the group. Besides the working ambiance, some things made the office a really pleasant place to go. For example, the team was united under the moose mascot and if we were late for the weekly group meeting, we had to bring cake to the next one. We often had cake.

Figure 1: A graceful moose, mascot of the Theoretical Microfluidic group

Every Friday, a meeting was organised with all the groups of the section. Then, a student, a professor or a visiting researcher talked about his work or a chosen subject. There were of course cakes.

3 Objectives of the internship

3.1 Initial definition of the contract

When I signed up my internship agreement, the objective of my project was not defined yet. I knew I was going to work on acoustic in microfluidic systems but the team was very open on the possibilities of my work there.

3.2 Analyse of the objectives of the intership

After a few days, Henrik and I decided to aim on the radiation force. This force is acting on a particle or a non water-miscible droplet in a microfluidic device and is due to the average of the second-order pressure in the ambient fluid. In the study of this force, the derivation relies on an important hypothesis. In this theory, all back reflections are neglected, which is of course impossible in reality. One paramount aim of my internship was to determine the influence of the reflections from the walls on the radiation force. More precisely, my different objectives were:

- Determining numerically a criterion for the scattering hypothesis to be valid
- Studying the influence of the walls on the radiation force on a particle in a homogenous ambiant fluid

3.3 Method

To understand the state-of-the-art, I first studied the theories of acoustic and of the radiation force. I mainly studied the papers Settnes and Bruus (2012) [1], Karlsen and Bruus (2015) [2], and Ley and Bruus (2017) [3]. I then learned how to use the software COMSOL Multiphysics (https://www.comsol.fr/comsol-multiphysics) in order to realise my simulations. The technical work will be presented below in section 6.

4 Theoretical Acoustic

4.1 Acoustic

Acoustic is the science which studies sound and mechanical waves propagating in matter. These waves are pressure and velocity perturbations wich transfer mechanical energy and momentum. As these waves are going to propagate in fluids in our study, we are going to briefly review the basic equations of Fluid Dynamic. A list of the properties of a fluid used in the report is found in Appendix 1.

The basic equations who rule Fluid Dynamic are the Navier–Stokes equations. There are three of them: the mass conservation, the momentum equation and the energy equation. In our study, we will neglect thermal effects and then we are going to use only the first two ones,

$$\frac{\partial \rho}{\partial t} + \underline{\nabla} \cdot (\rho \underline{v}) = 0 \tag{1}$$

$$\rho \frac{\partial \underline{v}}{\partial t} + \rho(\underline{v} \cdot \underline{\nabla})\underline{v} = -\underline{\nabla} p + \eta \nabla^2 \underline{v} + \beta \eta \underline{\nabla}(\underline{\nabla} \cdot \underline{v}) \tag{2}$$

A harmonic dependance in time will be assumed for all the studied fields. By convenience, we will use the complex time notation $e^{-i\omega t}$, where ω is the angular frequency of the actuating wave. Therefore, the velocity, the pressure and the density will be seen as complex. The physical fields will be the real part of these complex fields. Moreover, as every studied terms, including boundary conditions, will have this time dependancy, this complex exponential will be omitted in both theory and simulation.

4.2 Perturbation theory: introduction

The radiation force is an effect due to the time-averaged second-order pressure. In that way, we are going to see in the next subsections the order decomposition of the velocity, the pressure and the density, in order to get the order decomposition of the Navier–Stokes equations.

The zeroth order will represent the behaviour of the ambiant fuid without any wave propagating in it. The higher orders, representing the tiny perturbations, will be triggered by the wave whose amplitude is minute. The fluid will be considered quiescent before the presence of any wave (which implies $\underline{v}_0 = \underline{0}$).

We will show that the first order pressure is following a wave equation. We will then aim on the second-order pressure in order to study the radiation force.

4.3 Perturbation theory: first order decomposition and the Helmoltz equation

Here is the first order decomposition:

$$\underline{v} = \underline{0} + \underline{v}_1 \tag{3}$$

$$p = p_0 + p_1 \tag{4}$$

$$\rho = \rho_0 + \rho_1 \tag{5}$$

Moreover, we have the equation of state (see Appendix 1):

$$p_1 = c_0^2 \rho_1 \tag{6}$$

Including (3),(4) and (5) into (1) and (2), we get the first-order decomposition of Navier–Stokes equations:

$$\frac{\partial \rho_1}{\partial t} + \rho_0 \underline{\nabla} \cdot (\underline{v}_1) = 0 \tag{7}$$

$$\rho_0 \frac{\partial \underline{v}_1}{\partial t} = -\underline{\nabla} p_1 + \eta \nabla^2 \underline{v}_1 + \beta \eta \underline{\nabla}(\underline{\nabla} \cdot \underline{v}_1) \tag{8}$$

A single equation for ρ_1, ie for p_1, is obtained by inserting (8) in the time derivative of (7):

$$-\frac{\omega^2}{c_0^2} p_1 - \nabla^2 p_1 + (1+\beta)\eta \nabla^2 (\underline{\nabla} \cdot \underline{v}_1) = 0 \tag{9}$$

Then, we get:

$$-\frac{\omega^2}{c_0^2}p_1 = \left[1 - \frac{i\omega(1+\beta)\eta}{c_0^2\rho_0}\right]\nabla^2 p_1 \tag{10}$$

and:

$$-\frac{1}{1-\frac{i\omega(1+\beta)\eta}{c_0^2\rho_0}}\frac{\omega^2}{c_0^2}p_1 = \nabla^2 p_1 \tag{11}$$

Considering that $\frac{i\omega(1+\beta)\eta}{c_0^2\rho_0} \approx 10^{-5}$, we get to:

$$\left[1 + \frac{i\omega(1+\beta)\eta}{c_0^2\rho_0}\right]\frac{\omega^2}{c_0^2}p_1 = \nabla^2 p_1 \tag{12}$$

which is the Helmoltz equation:

$$\nabla^2 p_1 = -k^2 p_1 \tag{13}$$

k is the complex wavenumber. We have $k = k_0(1+i\Gamma)$ where $k_0 = \frac{\omega}{c_0}$ is the real wavenumber, modelising the propagation of the wave, and $\Gamma = \frac{(1+\beta)\eta\omega}{2\rho_0 c_0^2}$ is the damping factor. The last one has been and will be supposed minute in the bulk ($\Gamma \approx 10^{-5}$ with our parameters), it can often be neglected.

4.4 Irrotational hypothesis

Before looking at the second-order equations, we have to talk about another hypothesis we are going to make. As we will study pressure acoustic fields, we are going to do an assumption wich is going to be useful for our boundary conditions. We are going to neglect the rotational part of the velocity. To be clear, we have:

$$\nabla^2 \underline{v}_1 = \underline{\nabla}(\underline{\nabla}\cdot\underline{v}_1) - \underline{\nabla}\times(\underline{\nabla}\times\underline{v}_1) \tag{14}$$

Our assumption consists on negligting the rotational term: $\underline{\nabla}\times(\underline{\nabla}\times\underline{v}_1)$. This assumption is assimilating the velocity to its irrotanional compressible part, neglecting is non-divergent rotational one. In that way, the first order momentum equation (8) can be approximated by:

$$\rho_0\frac{\partial\underline{v}_1}{\partial t} = -\underline{\nabla}p_1 + (1+\beta)\eta\underline{\nabla}(\underline{\nabla}\cdot\underline{v}_1) \tag{15}$$

and using the first order mass conservation (7), we get a relation between the velocity and the pressure:

$$-i\omega\rho_0\underline{v}_1 = -\underline{\nabla}p_1 + i\omega\frac{(1+\beta)\eta}{\rho_0 c_0^2}\underline{\nabla}p_1 \tag{16}$$

ie:

$$\underline{v}_1 = -\frac{i}{\omega\rho_0}(1+i\Gamma)^2\underline{\nabla}p_1 \tag{17}$$

This asumption gives us simple boundary conditions for the pressure field using the velocity ones. The velocity field is going to be highly influenced in the narrow viscous boundary layer by this assumption but it is just a minor approximation on the pressure field, wich is the one we are going to study.

This asumption neglects the boundary viscous layer, as the shear is not considered in the fluid. The viscosity will only be modeled by the "bulk" damping factor. In this case, we do not have the no slip conditions ($\underline{v} = \underline{0}$) but the normal velocity conditions ($\underline{v}\cdot\underline{n} = 0$).

The "bulk" damping factor is usually very low compared to the "shear" damping factor, wich is the one we measure in reality. We will use this fact further in section 6.

We will use this hypothesis everywhere in our simulations and our theory, except when we will calcul one of the scattering coefficient (see Appendix 2).

4.5 Perturbation theory: second-order decomposition and radiation force

4.5.1 Definition

The radiation force is due to the time average of the second-order pressure in the acoustic field due to the scattering of an acoustic wave by the particle or the droplet. The particle, whose radius a is far lower than the wavelength λ of the incident wave, is going to act like a scattered point.

The radiation force is defined as the time-averaged effect of the fluid stress on the particle. The choice of the time average can be explained by two reasons:

- The particle is going to be moved by the first-order effect but this effect does only make it oscillate over a period: the time average of a first order variable is zero. Only the non-linear second-order effect will make it draft.
- Moreover, we often only observe experimentally the second-order quasi-steady drift effect, whose timescale is larger than the oscillating effect of the first order.

In our further derivation, we will consider the fluid inviscid, by convenience. We will make the main hypothesis to be discussed in the report that all back reflections of the scattering wave are neglected. We will neglect all the possible body forces and all thermal effects.

4.5.2 A general expression

We can obtain a useful expression for the radiation force considering an arbitrary static volum domain Ω_1 containing the particle Ω. The surfaces of the domains will respectively be called $\partial\Omega_1$ and $\partial\Omega$.

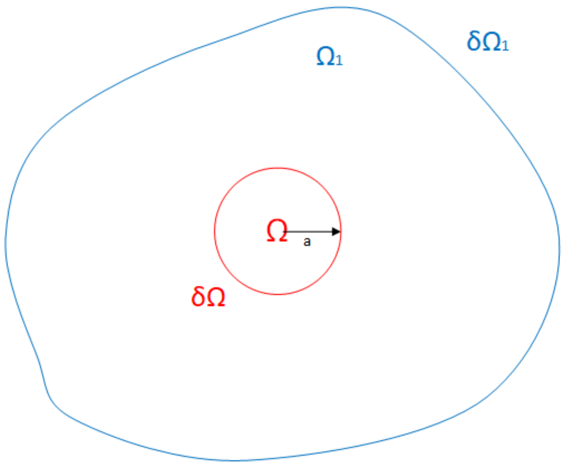

Figure 2: The particle Ω within an arbitrary volume domain Ω_1

If we apply Newton's second law on the fluid contained between the two surfaces, we have:

$$\frac{\mathrm{d}\underline{P}}{\mathrm{d}t} = \int_{\partial\Omega_1} [\underline{\underline{\sigma}} - \rho\underline{v} \otimes \underline{v}] \cdot \underline{n} \ \mathrm{d}S + \int_{\partial\Omega} \underline{\underline{\sigma}} \cdot (-\underline{n}) \ \mathrm{d}S \tag{18}$$

where $\underline{P}$ is the momentum of the system, $\underline{\underline{\sigma}}$ is the stress tensor and $\underline{n}$ is the normal vector going out of the surface $\partial\Omega_1$. As the time average of a total time derivative is zero in time-periodic systems, we get:

$$\underline{F_{\text{rad}}} = \left\langle \int_{\partial\Omega} \underline{\underline{\sigma}} \cdot \underline{n} \ \mathrm{d}S \right\rangle = \left\langle \int_{\partial\Omega_1} [\underline{\underline{\sigma}} - \rho\underline{v} \otimes \underline{v}] \cdot \underline{n} \ \mathrm{d}S \right\rangle \tag{19}$$

where the angled brackets represents the time average over a period.

4.5.3 second-order decomposition

Now we are going to study the second-order Navier–Stokes equations to link the second-order pressure to the first order terms. Here is the second-order decomposition:

$$\begin{aligned} \underline{v} &= \underline{0} + \underline{v}_1 + \underline{v}_2 && (20) \\ p &= p_0 + p_1 + p_2 && (21) \\ \rho &= \rho_0 + \frac{p_1}{c_0^2} + \rho_2 && (22) \end{aligned}$$

and then we get the second-order time-averaged equations:

$$\begin{aligned} \rho_0 \Big\langle \nabla(\underline{v}_2) \Big\rangle &= -\Big\langle \nabla(\rho_1 \underline{v}_1) \Big\rangle && (23) \\ \Big\langle \rho_1 \frac{\partial \underline{v}_1}{\partial t} \Big\rangle + \rho_0 \Big\langle (\underline{v}_1 \cdot \underline{\nabla}) \underline{v}_1 \Big\rangle &= -\Big\langle \underline{\nabla} p_2 \Big\rangle && (24) \end{aligned}$$

Some terms yielded to 0 because the time average of a first-order term is zero and because we neglected viscosity. Then, (24) leads to, using (8) with no viscosity term:

$$\Big\langle p_2 \Big\rangle = \frac{1}{2}\kappa_0 \Big\langle p_1^2 \Big\rangle - \frac{1}{2}\rho_0 \Big\langle v_1^2 \Big\rangle \tag{25}$$

A new formula for the radiation force occurs, using (19), (25), the fact that the time average of a first order variable is zero and the fact that zeroth order variables are constant:

$$\underline{F}_{\mathrm{rad}} = -\int_{\partial\Omega_1} \mathrm{d}a \left[\frac{1}{2}\kappa_0 \Big\langle p_1^2 \Big\rangle \underline{n} - \frac{1}{2}\rho_0 \Big\langle v_1^2 \Big\rangle \underline{n} + \rho_0 \Big\langle (\underline{n}.\underline{v}_1)\underline{v}_1 \Big\rangle \right] \tag{26}$$

4.5.4 Scattering theory

The last step consists on using the scattering theory to find a new expression of the radiation force, depending on two scattering coefficients f_0 and f_1, depending themselves of the properties of the particle and of the ambient fluid.

As a reminder, the particle, wich radius a is minute compared to the wavelength λ of the incident acoustic wave, is going to be a scattered point for this one. The first order variables will be decomposed in an incident field and a scattered one:

$$\underline{v}_1 = \underline{v}_{\mathrm{in}} + \underline{v}_{\mathrm{sc}} \tag{27}$$

According to (8), if we neglect the viscosity, the velocity can be written as the gradient of a potential ϕ:

$$\underline{v}_1 = \underline{\nabla}(\phi_1) = \underline{\nabla}(\phi_{\mathrm{in}}) + \underline{\nabla}(\phi_{\mathrm{sc}}) \tag{28}$$

and we have:

$$p_1 = i\omega\rho_0\phi_1 = i\omega\rho_0(\phi_{\mathrm{in}} + \phi_{\mathrm{sc}}) \tag{29}$$

Before inserting this new decomposition in the radiation force expression, we have to study the scaterred potential ϕ_{sc} using a multipole expansion.

As we are free to choose any domain Ω_1, we can choose a sphere of radius r_1, having the same center as the particle. We are going to choose $r_1 \gg \lambda$ to be in the so called far field region. In that case, the monopole component and the dipole component of the scattered potential dominate:

$$\phi_{\mathrm{sc}} \approx \phi_{\mathrm{mp}} + \phi_{\mathrm{dp}} \tag{30}$$

- The monopole component is due to the oscillatory compressibility of the particle
- The dipole component is due to its oscillatory center-of-mass motion

In general, these two components have these expressions:

$$\phi_{\text{mp}}(\underline{r},t) = \frac{1}{r}\, b(\underline{r}, t - \frac{r}{c_0}) \tag{31}$$

$$\phi_{\text{dp}}(\underline{r},t) = \underline{\nabla}\cdot\left[\frac{1}{r}\,\underline{B}(\underline{r}, t - \frac{r}{c_0})\right] \tag{32}$$

where b and $\underline{\text{B}}$ are two functions. We can notice that, as we are in the far field region, the potential components are time-retarded.

In the first order scattering theory, the scattered potential has to be proportional to the incident one. Using the only relevant physical fields, we have:

$$\phi_{\text{sc}} = -f_0 \frac{a^3}{3\rho_0 r} \frac{\partial \rho_{\text{in}}(\underline{r}, t - \frac{r}{c_0})}{\partial t} - f_1 \frac{a^2}{2} \underline{\nabla}\cdot[\frac{1}{r}\, \underline{v}_{\text{in}}(\underline{r}, t - \frac{r}{c_0}] \tag{33}$$

f_0 and f_1 are the scattering coefficients. We have added the radius of the particle a, the density of the fluid ρ_0 and the partial time derivative in order to get the right unit of the potential. The coeficients $\frac{1}{3}$ and $\frac{1}{2}$ are added for later convenience.

4.5.5 Final expression

According to (26), the radiation force is a sum of terms wich are all proportional to the square of $\phi_1 = \phi_{\text{in}} + \phi_{\text{sc}}$. This will lead to three kind of terms:

- Terms proportional to ϕ_{in} squared. They will yeld to 0 because they do not contain any information about the scattering.
- Terms proportional to ϕ_{sc} squared, therefore proportional to a^6. They will be negligible compared to the third kind of terms.
- Terms proportional to the product $\phi_{\text{in}}\phi_{\text{sc}}$, proportional to a^3. They are the dominant terms of the radiation force. We will only keep them in the further derivation.

Keeping only the mixed product terms in the expression (26), we have:

$$F_{\text{rad}} = -\int_{\partial\Omega_1} \mathrm{d}a \left[\kappa_0 \left\langle p_{\text{in}} p_{\text{sc}} \right\rangle \underline{n} - \rho_0 \left\langle \underline{v}_{\text{in}}.\underline{v_{\text{sc}}} \right\rangle \underline{n} + \rho_0 \left\langle (\underline{n}.\underline{v}_{\text{in}})\underline{v_{\text{sc}}} \right\rangle + \rho_0 \left\langle (\underline{n}.\underline{v_{\text{sc}}})\underline{v}_{\text{in}} \right\rangle \right] \tag{34}$$

Then, using Gauss theorem and simplifying:

$$\underline{F}_{\text{rad}} = -\int_{\Omega_1} \mathrm{d}r \left[\rho_0 \left\langle \underline{v}_{\text{in}} (-\frac{1}{c_0^2}\frac{\partial^2 \phi_{\text{sc}}}{\partial t^2} + \nabla^2 \phi_{\text{sc}} \right\rangle \right] \tag{35}$$

We can see that the d'Alembert operator appears. This operator is going to act on the time-retarded monopole and on the time-retarded dipole components of the scattering potential. It will yield them to a point charge distribution located in the center of the domain, ie the position of the center the particle:

$$-\frac{1}{c_0^2}\frac{\partial^2 \phi_{\text{sc}}}{\partial t^2} + \nabla^2 \phi_{\text{sc}} = f_0 \frac{4\pi a^3}{3\rho_0}\frac{\partial \rho_{\text{in}}}{\partial t} + f_1 2\pi a^3 \underline{\nabla}\cdot \underline{v}_{\text{in}} \tag{36}$$

where ρ_{in} and $\underline{v}_{\text{in}}$ are evaluated in the position occupied by the center of the particle.

Finally, we get another expression for the radiation force, after a few manipulations:

$$\underline{F}_{\text{rad}} = -\pi a^3 \left[\frac{2}{3}\kappa_0 \mathrm{Re}(f_0^* p_{\text{in}}^* \underline{\nabla} p_{\text{in}}) - \rho_0 \mathrm{Re}(f_1 \underline{v}_{\text{in}}^* \cdot \underline{\nabla}\underline{v}_{\text{in}})\right] \tag{37}$$

where the star means the complex conjugate. The two scaterring coefficients are equal to :

$$f_0 = 1 - \frac{\kappa_p}{\kappa_0} \tag{38}$$

$$f_1 = \frac{2[1-\gamma(\delta)](\frac{\rho_p}{\rho_0} - 1)}{2\frac{\rho_p}{\rho_0} + 1 - 3\gamma(\delta)} \tag{39}$$

where γ is a function of the viscous layer lenghtscale δ (to calcul the scattering coefficients, we do not use the irrotational or the inviscid hypothesis). In Appendix 2, you will find the derivation of these two formulas and the form of γ.

4.6 Resonnances in 1D

In this subsection, we will study an exemple of situation which higlights the resonnance phenomena. This example will be very useful in our further study.

We will study here an 1D situation (the velocity is therefore a scalar). A fluid is contained between two walls located respectively at $x = \frac{-L}{2}$ and $x = \frac{L}{2}$. These walls are vibrating in phase at the angular frequency ω, but the amplitude of these vibrations d_0 is minute, so they will be considered steady in the the referential of study.

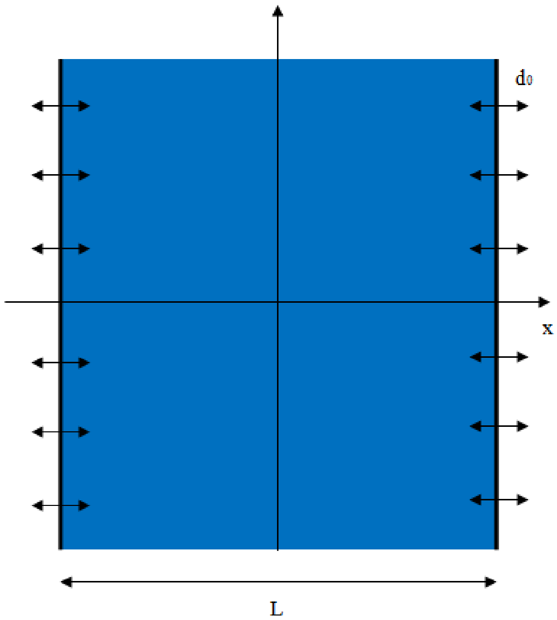

Figure 3: Figure of the situation. The fluid is represented in blue.

The vibration effect will then be modeled by these boundary conditions (as a reminder, the $e^{-i\omega t}$ is omitted):

$$v_1\Big(\pm\frac{1}{2}L\Big) = \omega d_0 \tag{40}$$

As we saw in the previous subsection, the first-order variables are following a Helmoltz equation. Therefore, the only possible wavenumbers for a single angular frequency in 1D are: $\pm k = \pm\frac{\omega}{c_0}(1+i\Gamma)$. The velocity is therefore a sum of these two modes:

$$v_1(x) = V_+e^{ikx} + V_-e^{-ikx} \tag{41}$$

The boundary conditions are imposing that v_1 must be even. The only possible case is that $V_+ = V_-$, so that a cosine can appear. Only standing waves are allowed to exist in this case:

$$v_1(x) = V_+e^{ikx} + V_-e^{-ikx} = V_+(e^{ikx} + e^{-ikx}) = \frac{V_+}{2}\cos(kx) \tag{42}$$

By using one of the two boundary conditions (40), we find that:

$$V_+ = V_- = \frac{2}{\cos(k\frac{L}{2})}\omega d_0 \tag{43}$$

so:

$$v_1(x) = \frac{\omega d_0}{\cos(k\frac{L}{2})}\cos(kx) \tag{44}$$

and the pressure, through equation (17), has the form:

$$p(x) = \frac{i\omega^2 \rho_0 d_0}{k(1+i\Gamma)^2 \cos(k\frac{L}{2})} \sin(kx) \tag{45}$$

It will exists some values of k so that the pressure reaches a peak. These values correspond to the resonnances. In this cases, the wvenumbers corresponding to the modes are:

$$k = \frac{(2n+1)\pi}{L}(1+i\Gamma)$$

where n is an integer.

5 Numerical tools

5.1 Finite element and Weak form

As a reminder, the aim of the finite element method is to discretize a physical fields by expanding it in a set of localized functions called the test functions. Each of these are associated with a geometrical node of the numeric mesh. For example, a physical field $g(x)$ will be expanded in that way:

$$g(\underline{r}) = \sum_n c_n \widehat{g}_n(\underline{r}) \tag{46}$$

where n is the number of nodes of the mesh and $\widehat{g}_n$ are the test functions.

These functions, usually polynomial, are equal to 1 on their associated node and vary to yield to 0 on the neighbouring nodes. They are also equalled to 0 further.

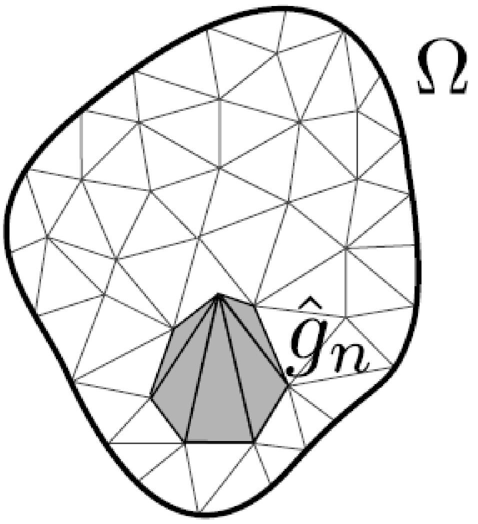

Figure 4: An example of linear test functions on a 2D domain

This discretization will create a numeric defect D.

To be consistent, the Theoretical Microfluidics Group chose the following convention. All equations will be written as continuity equations:

$$\underline{\nabla} \cdot \underline{J} = F \tag{47}$$

where $\underline{J}$ and F, wich depend of $g(\underline{r})$, are discretized. This is not very restrictive because many of physical equations can easily be written in this shape, and the above-mentionned numeric defect is $D = \underline{\nabla} \cdot \underline{J} - F$. In order to minimize this defect, we have to project it on a set of functions and put it to zero. The Galerkin method consists on projecting this defect on the test functions themselves. We have so, for every n:

$$\int_\Omega D\widehat{g}\mathrm{d}V = 0 \tag{48}$$

so:

$$\int_\Omega \left(\underline{\nabla} \cdot \underline{J}\widehat{g}_n - F\widehat{g}_n\right) \mathrm{d}V = 0 \tag{49}$$

ie, using an integration by parts:

$$\int_\Omega \left(\underline{\nabla} \cdot (\underline{J}\widehat{g}_n) - \underline{J}.\underline{\nabla}(\widehat{g}_n) - F\widehat{g}_n\right) \mathrm{d}V = 0 \tag{50}$$

and finally, by using the Gauss theorem, the Neumann conditions naturally appear:

$$\int_{\partial\Omega} \underline{J}.n\widehat{g}_n \;\mathrm{d}a + \int_\Omega \left(-\underline{J}.\underline{\nabla}(\widehat{g}_n) - F\widehat{g}_n\right) \mathrm{d}V = 0 \tag{51}$$

This integral form is called the weak form.

5.2 COMSOL Multiphysics

COMSOL Multiphysics is a simulation software based on finite element method. It has a wide range of options and permit to easily modelise physical situations.

We are not going to use one of its numerous prefabricated modules. In order to have the absolute control on the equations, we are going to use the weak form module. The software will permit us of implementing the volume terms of (51) with this syntax:

$$-\mathrm{test}(g_x) * Jx - \mathrm{test}(g_y) * Jy - \mathrm{test}(g) * F \tag{52}$$

where $test(g_x)$ and $test(g_y)$ are the x and y derivatives of $\widehat{g}_n$.

The Neumann boundary conditions will be added by an option called "Weak contribution". The software has a Cartesian logic. As our further simulations will be on a cylindrical device, we will have to add some corrective terms (see subsubsection 6.2.2).

5.3 The perfecty matched layer

As we will study situations where there will be no back reflections at the walls, we need to modelise the fact that outgoing waves are not reflected in a certain direction. To do it, we will use a mathematical tool: the perfectly matched layer (PML) [3]. A PML is domain acting as a perfect absorber of waves. In order to make this ideal absorbtion in this zone, we are going to modify one of the coordonate. In our cases, which will be in cylindrical coordonates, we will sometimes need a PML in the axial x-direction.The modification of the coordonate will be based on the real function s defined by:

$$s(x) = k_{PML}\left(\frac{x - L_0}{L_{PML}}\right)^2 \tag{53}$$

where k_{PML} (a positive integer) is the absorption coefficient, L_0 the beginning of the PML zone and L_{PML}, its length. We will multiply this function by booleans so that the zone is delimited by $x \in [L_0, L_0 + L_{PML}]$. This function will in that way be equal to 0 outside of the PML and increase as a parabol inside.

This modification will be implemented by changing all occurences in ∂x and dx:

- ∂x by $\frac{1}{1+is(x)}\partial x$
- $\mathrm{d}x$ by $(1 + is(x))\mathrm{d}x$

These modifications introduce an imaginary part and thus a damping for the outgoing waves. The values of k_{PML} and L_{PML} must be optimised to have a functionning PML and to make sure that the result is still physical (a too big absorbtion coefficient can induce non physical fields for example).

6 Technical Work

6.1 The studied system

6.1.1 Cylindrical system

In order to complete our objectives, we are going to study a cylindrical microdevice. The real device is composed by a glass structure filled with a liquid and some microparticles. Its aim is to control the particles thanks to the radiation force. In order to create this force, the system is actuated by acoustic waves generated by a piezoelectric device.

In some experiments, researchers used a lot of different geometries for these devices. The article [3], which gives 3D simulations of real experiments, simulates four different geometries. The cylindrical geometry we are going to modelise corresponds to the experiment described by Gralinski *et al.* [4]. In our simulations, the glass is going to be omitted and we will study only one particle located on the axis of the cylinder at the axial coordonate x_0.

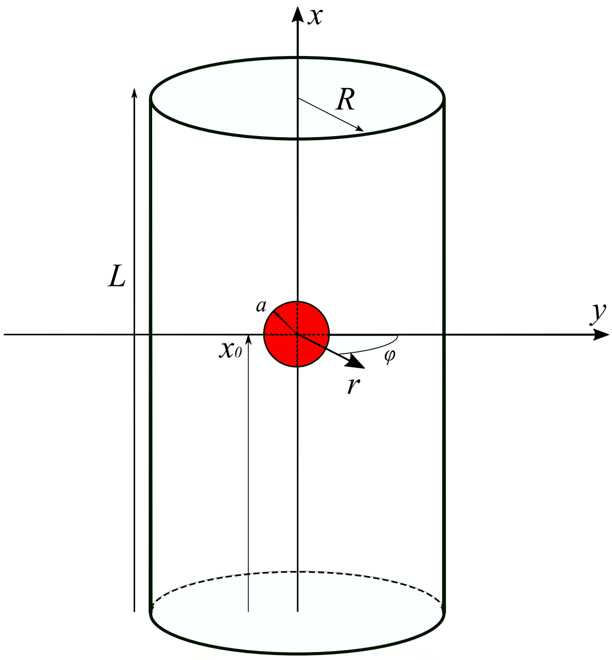

Figure 5: The studied microdevice: a cylindrical vertical structure of length L and radius R with a microparticle of radius a (red sphere) located on the axis at position x_0

We will obviously use the cylindrical coordonates in a given base $(\underline{e}_x, \underline{e}_r, \underline{e}_\phi)$ where the unit vector $\underline{e}_r$ is located by the angle ϕ compared to the unit vector $\underline{e}_y$ of the Cartesian base.

From now, we are going to assume that all the studied terms, including the boundary conditions, have a ϕ dependancy in $e^{im\phi}$ where m is an integer. This result is going to be verified in the next subsections for the incident pressure. This complex exponential will then be omitted for all the studied fields, as well as the time dependency.

In that way, we can study a 2D domain wich is "a slice" of our system for a given ϕ. This is this system we are going to use in our simulation.

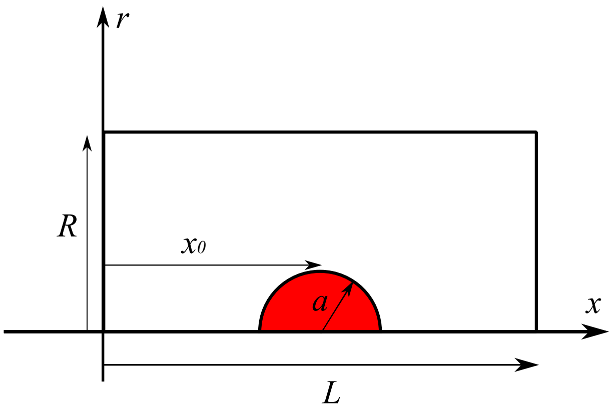

Figure 6: The cylindrical system sliced for a given ϕ

We can recover our complete system by doing a cylindrical revolution around the x-axis.

6.1.2 The incident pressure

We are actuating our system by making the walls located at $x = -\frac{L}{2}$ and $x = \frac{L}{2}$ vibrate, in the same way we saw in the 1D example in subsection 4.6. It will create a standing wave. In our simulation, we are going to modelise this incident pressure by an analytical function and we will study the acoustic field scattered by the particle. In this subsection, we are going to find the right shape of the incident presure, knowing that it has to follow the Helmoltz equation with vibrating walls boundary conditions.

General form of the Helmoltz equation's solutions in cylindrical coordonates: One takes a general function F=F(x,r,ϕ), following the Helmoltz equation of wavenumber k:

$$(\nabla^2 + k^2)F = 0 \tag{54}$$

We are going to do a variable decomposition to find the general form of the Helmoltz equation's solutions:

$$F(x, r, \phi) = A(x)B(r)C(\phi) \tag{55}$$

By including this form in the equation (54), we get:

$$\frac{\mathrm{d}^2 A(x)}{dx^2}B(r)C(\phi) + \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}(r\frac{\mathrm{d}B(r)}{\mathrm{d}r})A(x)C(\phi) + \frac{1}{r^2}\frac{\mathrm{d}^2 C(\phi)}{\mathrm{d}\phi^2}A(x)B(r) + k^2 A(x)B(r)C(\phi) = 0 \tag{56}$$

If we divide by $A(x)B(r)C(\phi)$, we have:

$$\frac{1}{A(x)}\frac{\mathrm{d}^2 A(x)}{\mathrm{d}x^2} + \frac{1}{rB(r)}\frac{\mathrm{d}}{\mathrm{d}r}(r\frac{\mathrm{d}B(r)}{\mathrm{d}r}) + \frac{1}{r^2 C(\phi)}\frac{\mathrm{d}^2 C(\phi)}{\mathrm{d}\phi^2} + k^2 = 0 \tag{57}$$

In that way, we can get, for $A(x)$:

$$\frac{\mathrm{d}^2 A(x)}{\mathrm{d}x^2} = -l^2 A(x) \tag{58}$$

Here, l is a constant wich physically represents the wavenumber in the direction $\underline{e}_x$. That's why we have chosen the constant of the right hand side of the equation in the form: "$-l^2$". We thus have for $B(r)$ and $C(\phi)$:

$$-l^2 + \frac{1}{rB(r)}\frac{\mathrm{d}}{\mathrm{d}r}(r\frac{\mathrm{d}B(r)}{\mathrm{d}r}) + \frac{1}{r^2 C(\phi)}\frac{\mathrm{d}^2 C(\phi)}{\mathrm{d}\phi^2} + k^2 = 0 \tag{59}$$

one can note:

$$\alpha^2 = k^2 - l^2 \tag{60}$$

In that way, we have:

$$\frac{1}{rB(r)}\frac{\mathrm{d}B(r)}{\mathrm{d}r}+\frac{1}{B(r)}\frac{\mathrm{d}^2B(r)}{\mathrm{d}r^2}+\frac{1}{r^2C(\phi)}\frac{\mathrm{d}^2C(\phi)}{\mathrm{d}\phi^2}+\alpha^2=0 \tag{61}$$

By multiplying by r^2, we get:

$$\frac{r}{B(r)}(\frac{\mathrm{d}B(r)}{\mathrm{d}r})+\frac{r^2}{B(r)}\frac{\mathrm{d}^2B(r)}{\mathrm{d}r^2}+\frac{1}{C(\phi)}\frac{\mathrm{d}^2C(\phi)}{\mathrm{d}\phi^2}+r^2\alpha^2=0 \tag{62}$$

And thus, we have, for $C(\phi)$:

$$\frac{\mathrm{d}^2C(\phi)}{\mathrm{d}\phi^2}=-m^2C(\phi) \tag{63}$$

where m is a constant wich physically represent the number of the angular mode in ϕ as we will see below.

Finally, we have, for $B(r)$:

$$r\frac{\mathrm{d}}{\mathrm{d}r}(r\frac{\mathrm{d}B(r)}{\mathrm{d}r})+(r^2\alpha^2-m^2)B(r)=0 \tag{64}$$

This is the well-known Bessel equation. To put it in a nutshell, we have:

$$\frac{\mathrm{d}^2A(x)}{\mathrm{d}x^2}+l^2A(x)=0, \tag{65a}$$

$$r\frac{\mathrm{d}}{\mathrm{d}r}(r\frac{\mathrm{d}B(r)}{\mathrm{d}r})+(r^2\alpha^2-m^2)B(r)=0, \tag{65b}$$

$$\frac{\mathrm{d}^2C(\phi)}{\mathrm{d}\phi^2}+m^2C(\phi)=0. \tag{65c}$$

with: $\alpha^2=k^2-l^2$.

In that way, we can find the form of one mode of F. For every mode, we have:

- $A(x)=A_1e^{ilx}+A_2e^{-ilx}$
- $B(r)=B_1J_m(\alpha r)+B_2Y_m(\alpha r)$ where J_m are the Bessel functions of the first kind and Y_m are the Bessel functions of the second kind.
- $C(\phi)=C_1e^{im\phi}+C_2e^{-im\phi}$

so, one mode can be written:

$$(A_1e^{ilx}+A_2e^{-ilx})(B_1J_m(\alpha r)+B_2Y_m(\alpha r))(C_1e^{im\phi}+C_2e^{-im\phi}) \tag{66}$$

and F is in reality the sum of an inifnity of these modes:

$$F(x,r,\phi)=\sum_{a,b,c}(A_{1a}e^{il_ax}+A_{2a}e^{-il_ax})(B_{1b,c}J_{m_c}(\alpha_{b,c}r)+B_{2b,c}Y_{m_c}(\alpha_{b,c}r))(C_{1c}e^{im_c\phi}+C_{2c}e^{-im_c\phi}) \tag{67}$$

As we can see, angular and radial modes are coupled through the Bessel functions.

First simplifications: In our case, the pressure $p(x,r,\phi)$ is following the Helmoltz equation of wavenumber k=$\frac{\omega}{c}(1+i\Gamma)$. Thus, we can say that:

$$p(x,r,\phi)=\sum_{a,b,c}(A_{1a}e^{il_ax}+A_{2a}e^{-il_ax})(B_{1b,c}J_{m_c}(\alpha_{b,c}r)+B_{2b,c}Y_{m_c}(\alpha_{b,c}r))(C_{1c}e^{im_c\phi}+C_{2c}e^{-im_c\phi}) \tag{68}$$

with:

$$\alpha_{b,c}^2=k_{a,b,c}^2-l_a^2 \tag{69}$$

We will use the symmetries and the boundary conditions of our situation to simplify the form of the pressure and to find all the possible wavenumbers. Every modes have to respect some conditions:

- According to our boundary conditions, the pressure has to be odd in x. In that way, for every mode (a,b,c), we can assume that: $A_{1a}e^{il_a x} + A_{2a}e^{-il_a x} = A_{0a}\sin(l_a x)$. Only standing waves are allowed.
- As we can choose the beginning of ϕ, we can choose that $C_{2c} = 0$.
- As we have a periodicity of 2π in ϕ, all m_c are integers. As they are integers, we shall not use the substrack c anymore and use m instead.
- As $\lim_{r\to 0} Y_m(r) = -\infty$ and in our case, the pressure is finite at r=0, we can assume that $B_{2b,m} = 0$

So the pressure can be written:

$$p(x,r,\phi) = \sum_{a,b,m} A_{0a}B_{1b,m}C_{1m}\sin(l_a x)J_m(\alpha_{b,m}r)e^{im\phi} \tag{70}$$

one can note: $P'_{a,b,m} = P_{a,b,m}A_{0a}B_{1b,m}C_{1m}$ and then:

$$p(x,r,\phi) = \sum_{a,b,m} P'_{a,b,m}\sin(l_a x)J_m(\alpha_{b,m}r)e^{im\phi} \tag{71}$$

Wavenumber in the direction $\underline{e_r}$ At each resonnance, the flux has to be zero at $r = R$, so for every (a,b,m) and for every (x,ϕ):

$$\alpha_{b,m}P'_{a,b,m}\sin(l_a x)J'_m(\alpha_{b,m}R)e^{im\phi} = 0 \tag{72}$$

Then:

$$\alpha_{b,m} = \frac{\gamma_{m,b}}{R}(1 + i\Gamma) \tag{73}$$

where $\gamma_{m,b}$ is the b^{th} root of the derivative of the m^{th} Bessel function in growing order.

Wavenumber in the direction $\underline{e_x}$: As we did in the section 4.6, we can find that:

$$l_a = (2a+1)\frac{\pi}{L}(1 + i\Gamma) \tag{74}$$

The only difference between the 1D case is that the vibrating velocity has to contain some information about m and b:

$$v_1\left(x = \pm\frac{L}{2}, r, \phi\right) = \omega d_0 J_m(\alpha_{b,m})e^{im\phi} \tag{75}$$

In that way, we also have access with the amplitude coefficient $P'_{a,b,m}$ of a given mode.

Dispersion relation We finaly have our complete dispersion relation, given by (60):

$$(\frac{\omega}{c_0})^2 = (\frac{\gamma_{m,b}}{R})^2 + ((2a+1)\frac{\pi}{L})^2 \tag{76}$$

With this relation, we can find the resonnance frequency of every modes. In our case, we are going to actuate only one mode, wich is the easiest to perform in real experiments: the mode 1-0-0 (1 in x, 0 in r, 0 in ϕ). This actuation will in that way be modeled by the analytical function: $p_{\text{in}} = P'_{1,0,0}sin(lx)$ with $l = \frac{\pi}{L}(1 + i\Gamma)$. In this mode, the wavelenght is twice the length of the device. The first simulation will consist on verifying that this actuation is correctly reflecting the experiment we want to modelise.

6.2 Numerical simulations and results

6.2.1 Mesh

Here we can see an example of mesh implemented in COMSOL for our simulations.

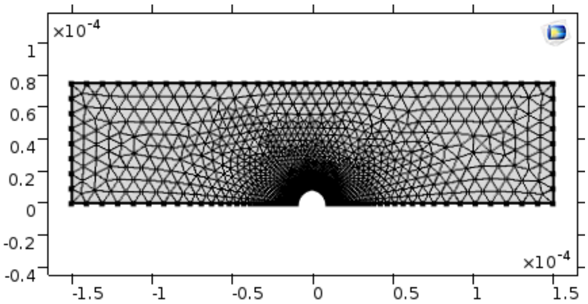

Figure 7: Mesh implemented

The mesh cells are triangular cells generated by the software. They will measure from $5\mu m$ to $10\mu m$ in the bulk and from $0.5\mu m$ to $1\mu m$ around the particle. To be able to mesh precisely without having a huge CPU time, the dimensions of the cylinder will be taken much lower than the one used in the real experiments of the article [4] ($L = 10mm$ and $R = 425\mu m$ in this article).

6.2.2 Helmoltz equation and the cylindrical coordonates corrective term for the scattered pressure

Here we are going to see the implementation of the Helmoltz equation for the scattered pressure p_{sc}, wich is the variable we are going to study in all our simulations (except the first one). We are currently using the cylindrical coordonates but COMSOL is based on a Cartesian logic. We must so adapt the equations to be able to use it in the software. It will add some corrective terms.

Here is the Helmoltz equation of wavenumber: $k = (1 + i\Gamma)\frac{\omega}{c}$ followed by the scattered pressure:

$$(\nabla^2 + k^2)p_{\text{sc}} \tag{77}$$

So, in cylindrical coordonates, taking into account the dependance in ϕ, we have:

$$(\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial}{\partial r}) - \frac{m^2}{r^2} + \frac{\partial^2}{\partial x^2} + k^2)p_{\text{sc}} = 0 \tag{78}$$

In order to implement this equation in the weak form, we are going to multiply it by the test function $\widehat{p_{\text{sc}}}$ and then integrate on all the volume of the cylindrical system Ω:

$$\int_\Omega \widehat{p_{\text{sc}}}(\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial}{\partial r}) - \frac{m^2}{r^2} + \frac{\partial^2}{\partial x^2} + k^2)p_{\text{sc}} r\mathrm{d}r\mathrm{d}\phi\mathrm{d}x = 0 \tag{79}$$

Then:

$$\int_\Omega \widehat{p_{\text{sc}}}(\frac{\partial}{\partial r}(r\frac{\partial}{\partial r}) - \frac{m^2}{r} + r\frac{\partial^2}{\partial x^2} + rk^2)p_{\text{sc}}\mathrm{d}r\mathrm{d}\phi\mathrm{d}x = 0 \tag{80}$$

By our symetry in ϕ, we get:

$$2\pi\int_{\Omega_{2D}} \widehat{p_{\text{sc}}}(\frac{\partial}{\partial r}(r\frac{\partial}{\partial r}) - \frac{m^2}{r} + \frac{\partial}{\partial x}(r\frac{\partial}{\partial x}) + rk^2)p_{\text{sc}}\mathrm{d}r\mathrm{d}x = 0 \tag{81}$$

where Ω_{2D} is the "slice" of cylinder for a given ϕ. To respect the formalism introduced in section 5, we can introduce:

- A current term $\underline{J} = 2\pi r \begin{pmatrix} \frac{\partial}{\partial r}(p_{\text{sc}}) \\ \frac{\partial}{\partial x}(p_{\text{sc}}) \end{pmatrix}$
- A body term $F = 2\pi(\frac{m^2}{r} - rk^2)p_{\text{sc}}$

The boundary conditions appears naturally thanks to the weak form, as we saw in section 5.

6.2.3 Study 1: The incident pressure

The first study consists of verifying the form of the incident pressure we want to modelise in the future files. In this simulation, the particle is not there yet and so there is not any scattered pressure field. We are going to study the pressure field generated by the wall vibrations and we are going to compare the shape of it with our theory developped above.

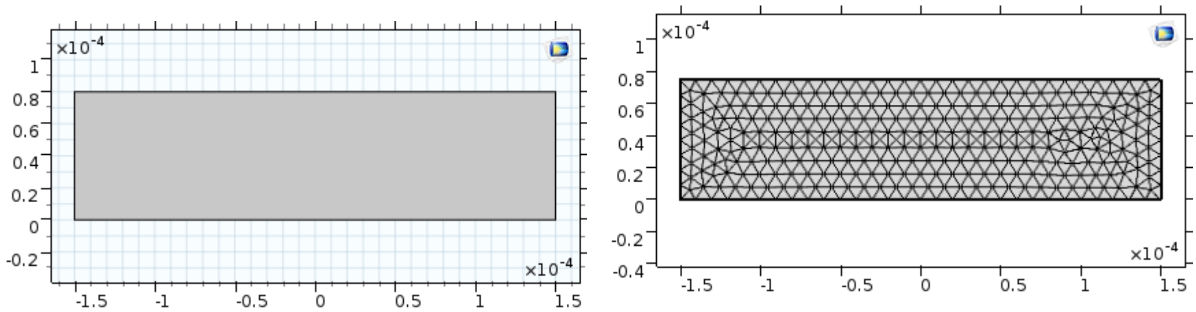

Figure 8: Geometry: $L = 300\mu m$ and $R = 75\mu m$

The walls vibrate at a certain resonnance frequency to excite the mode 1-0-0. We are going to verify the right shape of this field, and have access numerically to the amplitude coefficient of the mode P'_{1-0-0}.

To find the resonnance frequency, we make a parametric sweep of the vibration frequency around the theoretical value and we plot the acoustic energy density.

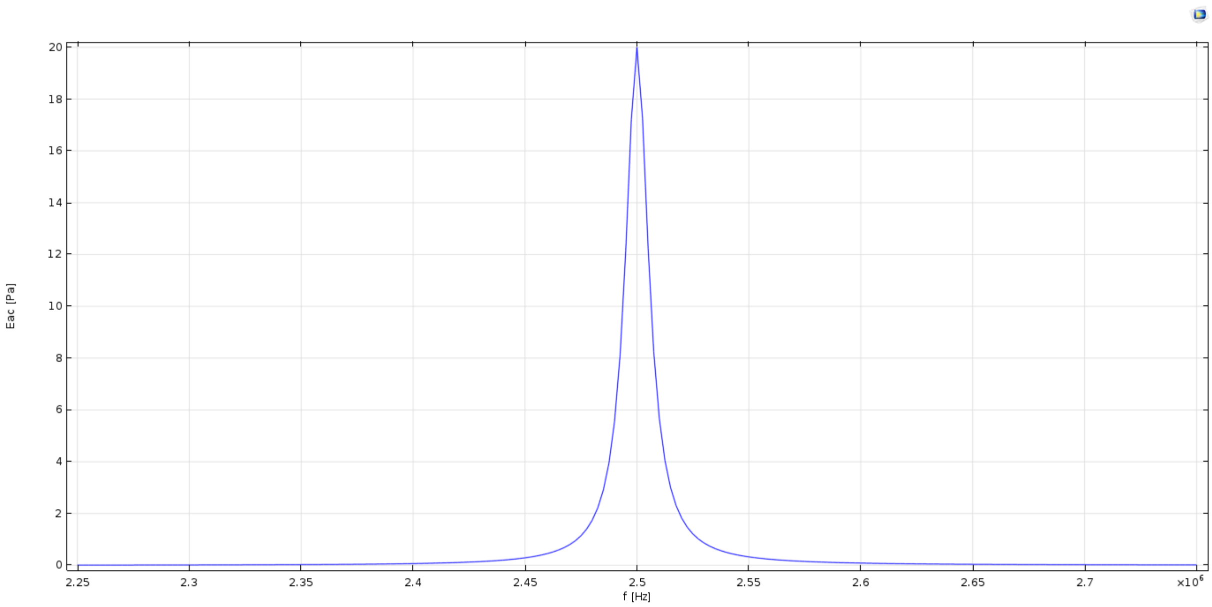

Figure 9: Acoustic energy density in function of the vibration frequency

This resonnance is visible on the above figure and the resonnance frequency is very close to the one calculated with the theory ($f_{1-0-0} = 2,5$MHz with our geometric parameters). The parametric sweep was made with 200 values from $2.25MHz$ to $2.75MHz$.

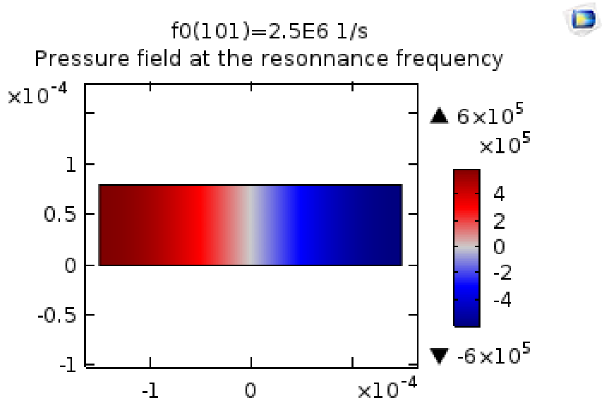

Figure 10: Pressure field(max:600kPa

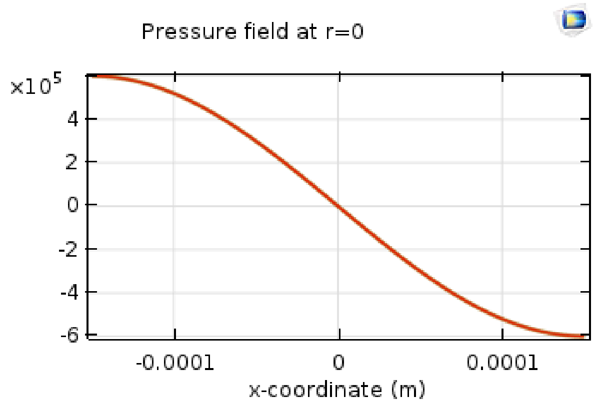

Figure 11: Pressure field at r=0

On this figures, we can see the pressure field. On the left figure, we can see the total pressure field and on the right figure, the pressure field at r=0 in function of x. The shape of the incident pressure is the one expected : $p_{\text{in}} = P^{'}_{1,0,0} sin(lx)$.

We now have all the tools to develop the actuation in our future studies. As the first-order equations will be linear, we are not going to look for the real physical amplitude of the actuation at each measure, we are going to normalize this to 10^5, by convenience. However, we know we could use the results of this subsection to get the physical amplitude of the further results. In the further studies, the walls will be considered as steady, because vibrations will already be "integrated" in the analytical function we have just found.

6.2.4 Study 2: Criterion of the validity of the scattering theory with an infinitely heavy and infinitely hard particle

Now we are studying the device with an infinitely hard and infinitely heavy particle in its center. This time, we are going to study the scattered pressure field. The incident pressure will be modeled by the normelised analytical function we have just verified.

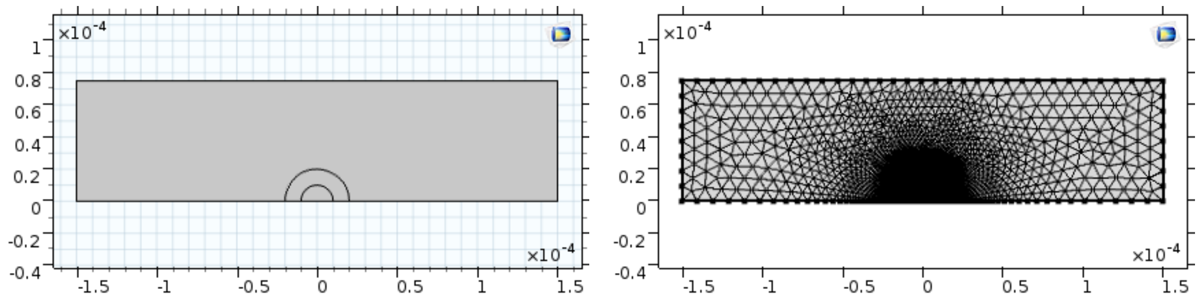

Figure 12: An example of geometry used in this study

We can see on the figure the particle (wich will act like a hard wall) and an arbitrary domain Ω_1 containing it. The boundary conditions are that the total first order pressure flux (the sum of the incident pressure flux and the scattered one) is zero at the walls and so also at the particle.

We choose that the criterion will concern the damping factor $\Gamma = \frac{(1+\beta)\eta\omega}{2\rho_0 c_0^2}$. We can identify two different regimes for a given case:

- At a low damping factor, the scattered wave is reflected at the walls and build up another resonnance. The scattered field then acquires the opposite phase compared to the incident one. We are not in the domain of validity of the scattering theory because the walls have a huge influence and the scattered wave is not outgoing.
- At an important damping factor, the scattered wave is not reflected enough by the walls to have a great influence and we can see the wave's outgoing behaviour. We are in the domain of validity of the theory.

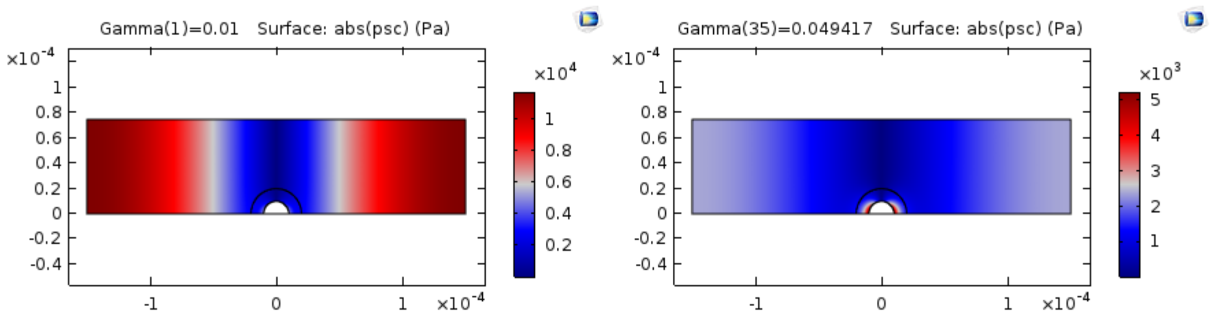

Figure 13: On the left, the absolute value of the scattered pressure field (max: $10kPa$ for $\Gamma = 0.01$ with $L = 300\mu m$ and $R = 75\mu m$ and on the right, the absolute value of the scattered pressure field (max: $5kPa$ for $\Gamma = 0.05$ with $L = 300\mu m$ and $R = 75\mu m$

Between this two regimes, when we rise the damping factor, the amplitude of the scattered wave, which has built up a resonnance, becomes lower and lower until it reachs the outgoing behaviour. As a choice for the criterion, we are going to define the critical damping factor Γ_c as the damping factor wich leads to:

$$max(|p_{\mathrm{sc}}|) = 0.2|p_{\mathrm{in}}|$$

In order to find this critical value, we are going to choose the position of the particle where the scattering (depending of the gradient of the incident pressure) will be maximal: $x_0 = 0$. This critical damping factor depends on parameters we have to determine. Let's use the Pi theorem to find non-dimensional numbers on wich Γ_c will depend. Here are the equations related to the experiment:

$$\begin{aligned}
(k^2 + \nabla^2)p_{\mathrm{sc}} &= 0 && \text{(82a)}\\
k &= \frac{\omega}{c}(1 + i\Gamma) && \text{(82b)}\\
\frac{\omega}{c_0} &= \frac{\pi}{L} && \text{(82c)}\\
\underline{\nabla} p_{\mathrm{sc}}(\underline{r_{wall}}) \cdot \underline{n} + \underline{\nabla} p_{\mathrm{in}}(\underline{r_{wall}}) \cdot \underline{n} &= 0 && \text{(82d)}\\
p_{\mathrm{in}} &= p_{\mathrm{a}} sin(kx) && \text{(82e)}
\end{aligned}$$

where :

- The first equation is the Helmoltz equation for the scattered pressure
- The second one is the definition of the complex wavenumber
- The third one is the fact that we are actuating the system at its mode 1-0-0
- The fourth one traduce the boundary conditions
- The last one is the analytical function of the incident pressure

In that way, we have : $\Gamma_c = f(L, R, a)$. The critical damping factor is only depending on the geometry of the device and of the particle.

We can then defined two non-dimensional numbers L/R and a/R so that:

$$\Gamma_c = f\left(\frac{L}{R}, \frac{a}{R}\right). \tag{83}$$

We are then going to modify the geometry to get the curves of the critical damping factor.

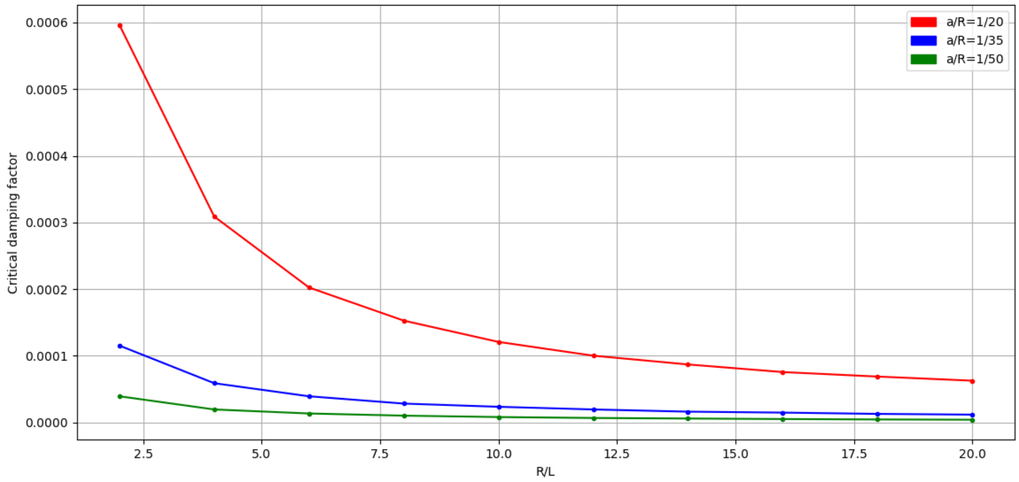

Figure 14: Critical damping factor Γ_c as function of the geometry of the device L and R as well as of the geometry of the particle a

For a given experiment with a cylindrical device and with our current actuation, we could use this curve to see what geometry we could use if we don't want to have the walls' influence. In a real case, the damping factor to compare with the critical value could be the "shear" damping factor, wich is far higher than the "bulk" one.

Let's use these curves with the experiment of the article [4]. In this experiment, the fluid used is water, the actuating frequency is around $1MHz$ and the geometric parameters are $L = 10mm$, $R = 425\mu m$ and $a = 5\mu m$. We have then: $\frac{L}{R} = 23$ and $\frac{a}{R} = \frac{1}{85}$. We are going to place the shear damping factor on the curves to see if the walls actually play a role or not. We have $\Gamma^s = 1.3\ 10^{-3}$.

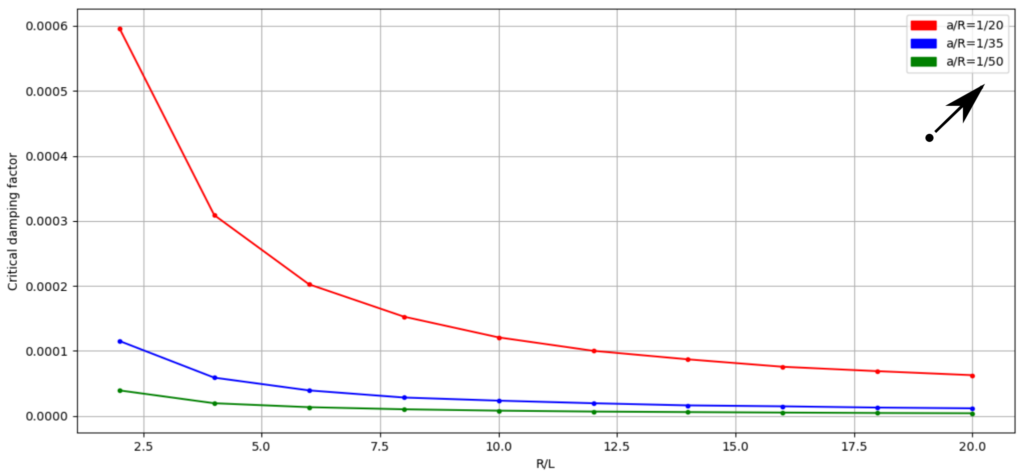

Figure 15: The experiment situation compared with the criterion. The actual experimental parameters are far outside the depicted interval, wich is indicated by the point and the black arrow in the top-right corner.

As we can see on the figure, the damping factor, located by the black point, is far higher than the critical curve wich would correspond to $\frac{a}{R} = \frac{1}{85}$. The walls do not play a role and the scattering theory can be used without any hesitation.

6.2.5 Study 3: Radiation force on a infinetily weighed and infinitely hot particle

In this simulation, we are going to see the effects of the walls on the radiation force. First, we are going to compare our simulation results to the ones obtained by the theory in the case of no back reflections.

On one hand, we make a simulation using PML (Perfectly matched layer, see section 5) zones in the $\underline{e}_x$ direction, so that we get a perfect absorption of the waves close to the walls. The criterion will be then verified whatever the value of the damping factor. The geometry will be $R = 75\mu m$ and $L = 300\mu m$. The actuation and the boundary conditions remain the same.

We implement the radiation force through the formula (26):

$$\underline{F}_{\mathrm{rad}} = -\int_{\partial\Omega_1} \mathrm{d}a \left[\frac{1}{2}\kappa_0\left\langle p_1^2\right\rangle\underline{n} - \frac{1}{2}\rho_0\left\langle v_1^2\right\rangle\underline{n} + \rho_0\left\langle(\underline{n}.\underline{v}_1)\underline{v}_1\right\rangle\right]$$

On the other hand, we use a Python program to get the curve of the theoretical radiation force. To get it, we use the formula issued of the scatering theory (37):

$$\underline{F}_{\mathrm{rad}} = -\frac{4\pi}{3}a^3\underline{\nabla}(\frac{1}{2}Re(f_0)\kappa_0\left\langle p_{\mathrm{in}}^2\right\rangle - \frac{3}{4}Re(f_1)\rho_0\left\langle v_{\mathrm{in}}^2\right\rangle)$$

As the particle is infinitely heavy and infinitely hot, the factors f_0 and f_1 are both equal to 1.We can compare the two curves.

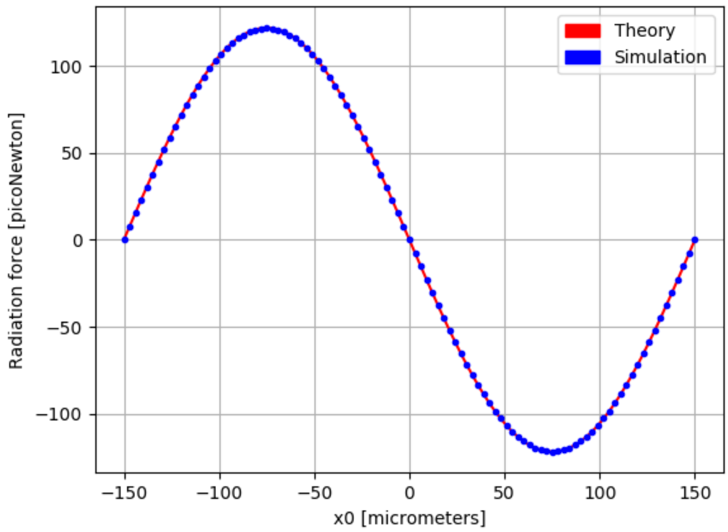

Figure 16: Comparison between the radiation force calculated with the formula issued of the scattering theory and the one obtained by the simulation with PML

As we can see on the figure, the result is very satisfying. We have the same shape (a sinusoidal with a wavelength equal to the double of the actuation's one) and the relative error between the two amplitudes is less than 1%. With the PML, our simulation is so verifying the theory.

We will now take off the PML to see what could be the influence of the walls for different values of the damping factor. For this geometry, the critical damping factor is of 5×10^{-3}.

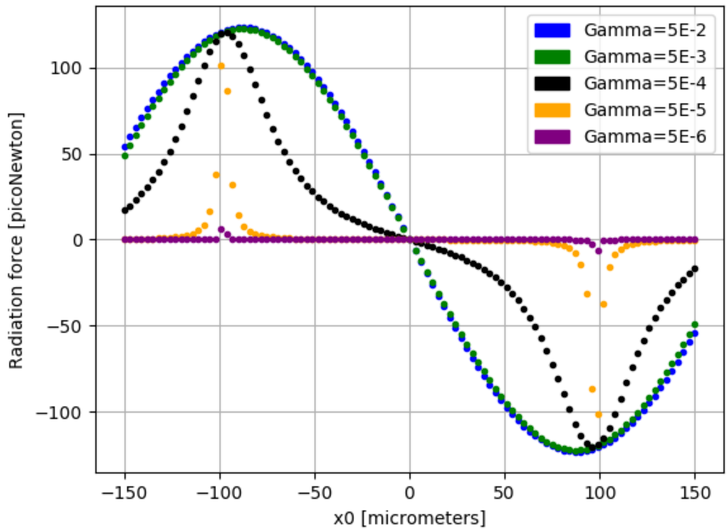

Figure 17: Radiation force on the infinitely hard and infinitely heavy particle for different values of the damping factor

As we can see on the figure, the walls are lowering the radiation force. With a low damping factor, the scattered waves build up a resonnance wich tend to cancel the incident field. Their interferences are just destroying each other, without creating any time average defect on the particle.

6.2.6 Study 4: Adding real properties

To define our criterion, we used an ideal particle ($\rho_p \to \infty$ and $\kappa_p = 0$).We could define a more general criterion, but it will also depend on the scattering coefficients f_0 and f_1. The graphical representation would be far more complicated and the curves far more time-consuming to get. In that way, we are going to reproduce the previous study to see if the fact that the particle have real properties will go in our way or not.

This simulation will be exactly the same as the one before but using a particle with a finite density ρ_p and on non zero compressibility κ_p. We will modelise the particle by a droplet, to avoid using solid mechanics. It will be a droplet of glycerol (with $\rho_p = 1300 kg/m^3$ and $\kappa_p = 2.20 \times 10^{-10} Pa^{-1}$). Here are the curves:

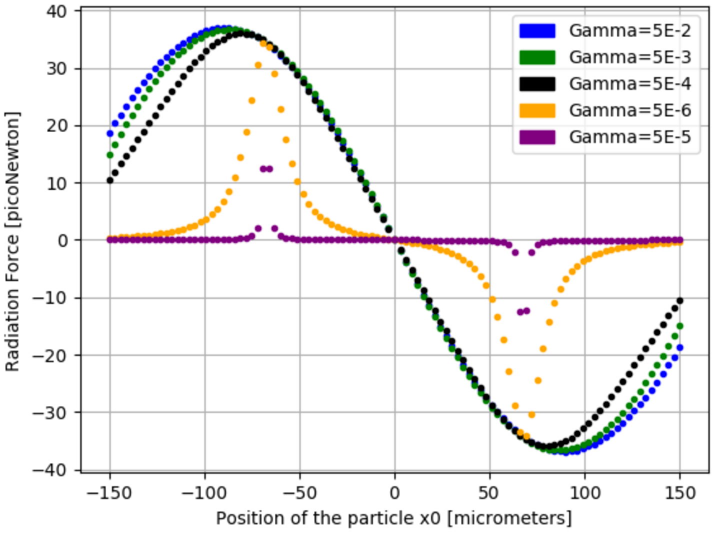

Figure 18: Radiation force on a droplet of glycerol for different values of the damping factor

As we can see on the figure, the radiation force tend to yield to 0 with a decreasing damping factor as before, but the critical damping factor seems to be lower (the curve for $\Gamma = 5\ 10^{-}3$ is less altered). When the particle is real, the scattering is not ideal, not complete. The fact that the particle is infinitely heavy and infinitely hard represents so the worst case if we don't want any effect of the walls. In that way, the criterion obtained with a perfect particle can be used for real particles because if a geometry satisfies the first one, it will satisfy the second.

7 Conclusion

7.1 Conclusion on the results

To conclude on this report, we defined a criterion on the damping factor in a "lab-on-chip" to determine if the walls were going to play a role on the scattering of the incident wave by a particle. We then saw that if this criterion is not respected, the walls were going to diminish on the radiation force exerced on the particle, making it yield to zero.

7.2 Mission completed?

If we look at the initial contract, I think I succeeded into completing my objectives. I would have wanted more time to study the case of a inhomogenous ambient fluid but I think that my results could help the researchers in the future.

7.3 Being a researcher

I was completely free on this project. Professor Bruus trusted me and I was able to understand many theoretical aspects on acoustofluidic. I must say I really loved this experience. It was my largest study project as a researcher, and it really made me want to go on to become a full-time researcher. That is why I am heading to do a PhD next year.

8 Appendices

8.1 Appendix 1: Basic properties of a fluid and Mathematical operators

8.1.1 Basic properties of a fluid

- ρ: Density of the fluid. It is the mass of the fluid per unit volume.
- η: The dynamic shear viscosity of the fluid. It is a measure of its resistance to gradual deformation induced by a shear stress.
- β: β is the ratio between the shear viscosity and the viscosity related to compressibiliy-induced stress.
- κ: Compressibility of the fluid. It is a measure of the relative volume change of the fluid as a response to a pressure actuation. This behaviour depends on if the actuation is adiabatic or isothermal. We can then define two compressibility coefficients: the isothermal one $\kappa_T = -\rho(\frac{\partial \rho}{\partial p})_T$ and the isentropic one $\kappa_s = -\rho(\frac{\partial \rho}{\partial p})_s$. We will use the isentropic one (in the report, we will denote $\kappa_0 = \kappa_s$)
- c_0: Speed of sound in the fluid. It is the distance travelled by a sound wave per unit time in the fluid. We have: $c_0 = \sqrt{\frac{1}{\rho \kappa_s}} = \sqrt{(\frac{\partial p}{\partial \rho})_s}$

8.1.2 Equation of state

In subsection 4.3, we use the equation of state (6) to find the first order equations. Here we are going to see the derivation of this formula. By doing a Taylor expansion of the pressure, function of the density and of the entropy, we get:

$$p(\rho, s) \approx p_0 + p_1 = p(\rho_0) + (\rho - \rho_0)(\frac{\partial p}{\partial \rho})_s$$

so we get :

$$p_1 \approx \rho_1 c_0^2$$

8.2 Appendix 2: Derivation of the scattering coefficients

In this subsection, we are going to calculate the scattering coefficients. We are going to use spherical coordonates with the base ($\underline{e_r}$, $\underline{e_\theta}$, $\underline{e_\phi}$) located at the instantaneous center of the particule. As it was said, we will not use the irrotational hypothesis here. In that way, the visous boundary layer cannot be neglected. Its lenght scale is denoted δ and we have:

$$\delta = \sqrt{\frac{2\eta}{\rho_0 \omega}} \tag{84}$$

We are then going to define three zones:

- the viscous boundary layer $r \in [a, a + 5\delta]$
- the near field region $a + 5\delta \ll r \ll \lambda$
- the far field region $r \gg \lambda$

Moreover, we will assume here that we have a symmetry in ϕ. The velocity of the particle will be denoted $\underline{v_p}$. In this coordonates, we have:

$$\underline{v_{\text{in}}} = v_{\text{in}}(\cos(\theta)\underline{e_r} - \sin(\theta)\underline{e_\theta}) \tag{85}$$

$$\underline{v_p} = v_p(\cos(\theta)\underline{e_r} - \sin(\theta)\underline{e_\theta}) \tag{86}$$

In the near field region, the potential components are going to depend on the instantaneous time variable t and not the retarded one $t - \frac{r}{c_0}$. In the near field region, (33) gives us:

$$\phi_{\text{sc}}(r,\theta) = \phi_{\text{mp}}(r) + \phi_{\text{sc}}(r,\theta) = -f_0 \frac{a^3}{3\rho_0 r}\frac{\partial \rho_{\text{in}}(t)}{\partial t} - f_1 \frac{a^2}{2}\underline{\nabla} \cdot [\frac{\underline{v_{\text{in}}}(t)}{r}] = -f_0 \frac{a^3}{3\rho_0 r}\frac{\partial \rho_{\text{in}}(t)}{\partial t} + f_1 \frac{a^2}{2} v_{\text{in}}(t)\frac{cos(\theta)}{r^2} \tag{87}$$

8.2.1 The monopole coefficient f_0

The monopole behaviour is the one of a steady compressible particle. The presence of the particle induce a mass rate of scattered fluid:

$$\frac{\partial m}{\partial t} = \int_{\partial\Omega} \underline{n}.(\rho_0 \underline{\nabla} \phi_{\text{mp}}) da = f_0 \frac{4\pi}{3} a^3 \frac{\partial \rho_{\text{in}}}{\partial t} \tag{88}$$

We also have:

$$\frac{\partial m}{\partial t} = \frac{\partial}{\partial t}[(\rho_0 + \rho_{\text{in}}(t))V_p(t)] \tag{89}$$

where $V_p(t)$ is the volume of the particle.
Using the definition of the compressibility, we get to:

$$\frac{\partial m}{\partial t} = (1 - \frac{\kappa_p}{\kappa_o})V_p(t)\frac{\partial \rho_{\text{in}}}{\partial t} \tag{90}$$

We then get:

$$f_0 = 1 - \frac{\kappa_p}{\kappa_o}$$

8.2.2 The dipole coefficient f_1

The dipole behaviour is the one of an incompressible particle moving in the fluid. We are going to match the velocity of the fluid in the near field region ($\underline{v_{\text{in}}} + \underline{\nabla}(\underline{\phi_{\text{sc}}})$) with the particle's one ($\underline{v_p}$) in order to find the scattering coefficent. In the boundary layer zone, the fluid will be supposed incompressible (the time it takes for an acoustic waves to propagate through this zone is much less than an oscillation). We will denote $\underline{v_{bl}}$, the first order velocity in this boundary layer. This velocity has to fulfil the no-slip condition:

$$\underline{v_{bl}}(a,\theta) = \underline{0} \tag{91}$$

Using an asymptotical matching at a distance r^* with $a + 5\delta \ll r^* \ll \lambda$, we have:

$$\underline{v}_{bl}(r^*, \theta) = (1 - f_1 \frac{a^3}{r^3}) \cos(\theta) \underline{e}_r + (1 + f_1 \frac{a^3}{2r^3})(-\sin(\theta)) \underline{e}_\theta \tag{92}$$

We can find the velocity of the particle by using Newton's second law:

$$-i\omega \frac{4}{3} \pi a^3 \rho_p v_p \underline{e}_x = \int_\partial \underline{\underline{\sigma}}^{bl} \cdot \underline{n}.\underline{e}_x \mathrm{d}a = 2\pi a^2 \int_{-1}^{1} \mathrm{d}(\cos(\theta))[\sigma^{bl}_{rr} r \cos(\theta) - \sigma^{bl}_{r\theta} \sin(\theta)] \tag{93}$$

where the stress tensor components are $\sigma_{rr} = -p_{bl} + 2\eta \frac{\partial v_r^{bl}}{\partial r}$ and $\sigma_{r\theta} = \eta(\frac{1}{r}\frac{\partial v_r^{bl}}{\partial \theta} + \frac{\partial v_\theta^{bl}}{\partial r} - \frac{v_\theta^{bl}}{r})$

We then have to determine the fields p_{bl} and $\underline{v}_{bl}$. In order to do this, we will use the fact that the fuid is considered incompressible in the boundary layer (which implies $\underline{\nabla} \cdot \underline{v}_{bl} = 0$).

Taking the divergence of the first order momentum equation (8), we get to the Laplace equation : $\nabla^2 p_{bl} = 0$. Since p_{bl} has to match with the dipole part in the near field region ($i\rho_0\omega(\phi_{\text{in}} + \phi_{\text{dp}})$), we get to:

$$p_{bl}(r, \theta) = i\rho_0\omega[r + \frac{a^3}{2r^2} f_1] v_{\text{in}} \cos(\theta) \tag{94}$$

For the velocity field, the incompressibility and the azimutal symmetry both leads to the fact $\underline{v}_{bl}$ can be written in function of the stream function $\Psi(r, \theta)$:

$$\underline{v}_{bl}(r, \theta) = \underline{\nabla} \times [\Psi(r, \theta) \underline{e_\phi}] \tag{95}$$

It can be shown that, by taking the rotation of the first order momentum equation, the stream function can be written as the sum of two terms Ψ_1 and Ψ_2 wich has to respect:

$$\nabla^2 \Psi_1 - \frac{\Psi_1}{r^2 \sin^2(\theta)} = 0 \tag{96}$$

$$\nabla^2 \Psi_2 - \frac{\Psi_2}{r^2 \sin^2(\theta)} = -q^2 \Psi_2 \tag{97}$$

We denoted $q = \frac{1+i}{\delta}$. It contains all the information about the viscosity. The solutions of these equations are:

$$\Psi_1 = A_1 r \cos(\theta) + A_2 \frac{\cos(\theta)}{r^2} \tag{98}$$

$$\Psi_2 = B h_1^1(qr) a v_{\text{in}} \sin(\theta) \tag{99}$$

where $h(s) = -\frac{i+s}{s^2} e^{is}$ is the Hankel function of the first kind of order 1. We can see that this function yield to 0 exponentially. In the near field region, outside of the boundary layer, this function is so equal to 0. We find the two constants A_1 and A_2 using the asymptotical matching conditions (Ψ_2 being equalled to 0 outside of the boundary layer):

$$\Psi_1(r, \theta) = [\frac{1}{2} r - f_1 \frac{a^3}{2r^2}] v_{\text{in}} sin(\theta) \tag{100}$$

So we can find the velocity in the boundary layer:

$$\underline{v}_{bl} = \underline{\nabla} \times (\Psi_1 + \Psi_2) 1 - \frac{f_1 a^3}{r^3} + 2qaB \frac{h_1^1(qr)}{qr}] \cos(\theta) v_{\text{in}} \underline{e}_r + [1 + \frac{f_1 a^3}{2r^3} + qaB \frac{1}{qr} \frac{\partial(s h_1^1(s))}{\partial s}(s = qr)](-\sin(\theta)) v_{\text{in}} \underline{e_\theta} \tag{101}$$

By inserting this formula of the velocity, with the pressure into the Newton's second law, and using the no slip conditions, we have three equations with three unknowns (f_1, v_p and B):

$$v_p = [1 - f_1 + 2B h_1^1(qa)] v_{\text{in}} \tag{102}$$

$$v_p = [1 + \frac{1}{2} f_1 + B \frac{1}{qr} \frac{\partial(s h_1^1(s))}{\partial s}(s = qa)] v_{\text{in}} \tag{103}$$

$$\frac{\rho_p}{\rho_0} v_p = [1 + \frac{1}{2} f_1 + +2B h_1^1(qa)] v_{\text{in}} \tag{104}$$

After resolving this system, using also the fact that $\frac{\partial(sh_1^1(s))}{\partial(s)} - 2h_1^1(s) = sh_0^1(s) - 3h_1^1(s)$ (with $h_0^1 = -\frac{i}{s}e^{is}$ the Hankel function of the first kinf of order 0), we get the result:

$$f_1 = \frac{2[1-\gamma(\delta)](\frac{\rho_p}{\rho_0} - 1)}{2\frac{\rho_p}{\rho_0} + 1 - 3\gamma(\delta)}$$

with $\gamma(\delta) = \frac{3h_1^1(qa)}{qah_0^1(qa)} = \frac{3\delta}{2a}[1 + i(1 + \frac{\delta}{a})]$

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