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Optimal design of silicon-based chips for piezo-induced ultrasound resonances in embedded microchannels

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Abstract

We present a variational formulation of the governing equations and introduce global indicators to describe the behavior of acoustofluidic devices driven at resonance frequencies by means of a piezoelectric transducer. The individuation of the correct Lagrangian densities for the different parts constituting the device (the piezo transducer, the silicon walls, the fluid-filled microchannel, and the glass lid) allows for the introduction of the weak formulation used in the finite element discretization of the equations describing the system in its oscillatory regime. Additionally, the knowledge of the Lagrangian density leads to the derivation of the correct structure of the Hamiltonian density, i.e. the energy density, which is important for the quantification of the energy content of the whole system and its individual parts. Specifically, the energy content of the embedded microchannel is quantified by means of the acoustofluidic yield η defined as the ratio between the energy in the channel and the total energy. From the standpoint of acoustophoretic application, the introduction of the acoustophoretic mean orientation allows us to identify the frequencies for which an acoustophoretic effect, i.e. the lateral motion of particle dragged by the axial main flow, is particularly strong. Finally, the connection between the mechanical and electrical degrees of freedom of the system is addressed. This is important for proper determination of the dissipated power, and it may lead to the detection of resonance states by means of purely electrical measurements. Numerical simulations and preliminary experimental results show some features of the model introduced.

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1. Introduction

Acoustophoretic devices represent an efficient and easy-to-set-up method for the manipulation of biological samples. Indeed, this method has been shown to be able to manipulate cell lines as well as micrometric-sized beads (1; 2), by simply using an embedded microfluidic channel, or a capillary, in connection with the presence of a piezoelectric actuator that in the simplest cases can be glued to the structure containing the micro-channel (3). Despite the advantages in using this kind of technique with respect to other manipulation methods, e.g. (di-)electrophoresis and magnetophoresis, the identification of optimal working frequencies is yet entrusted with the presence of the operator, who has to search manually for resonance frequencies that afterwards can be tracked with the aid of electric mea-

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surements. Furthermore, the design of acoustofluidic systems deserves additional investigations, since optimization of the geometric configuration of the device as well as the material properties can point out better ways to improve the effectiveness of the separation process and lead to a broadening of the range of applicability.

To this end, the present manuscript addresses objective global indicators that aid both the designer and the experimentalist to locate optimal working frequencies (4). The introduction of these global indicators is based upon a preliminary description of the equations governing the system in terms of Lagrangian densities. Specifically, the mechanical Lagrangian density features the parts of the system obeying to Helmoltz–Navier equation which describes elastic waves in the frequency domain. On the other hand, the acoustic Lagrangian density represents the propagation of acoustic pressure wave in the inviscid fluid, meaning that the corresponding governing equation is the Helmoltz wave equation for the pressure. Finally, the electro-mechanical Lagrangian density describes elastic waves in the piezoelectric element driven by the coupling to the dielectric behavior of the material in the presence of an imposed potential difference.

Addressing the exact form of the Lagrangian densities is important in two regards. First, the weak formulation of the governing equations for the finite element implementation stems directly from the individuation of the Lagrangian densities. This is important in the development of numerical methods that can be systematically checked by means of physical considerations. Second, the Hamiltonian density can be retrieved by splitting of the Lagrangian density in the kinetic and potential energy densities and summing them. The Hamiltonian density is important for the quantification of the system energy in all of the subsequent quantities, and it can be used to characterize the system both from the mechanical and electrical point of views.

Table 1. List of symbols.

ρ	Density	c	Speed of sound
$\boldsymbol{\varepsilon}$	Dielectric tensor	$\boldsymbol{P}$	Piezoelectric coupling matrix
$\boldsymbol{\Sigma}$	Stiffness tensor		
$\mathscr{L}$	Lagrangian density	$\mathscr{H}$	Hamiltonian density
$\boldsymbol{u}$	Displacement	p	Pressure
$\boldsymbol{\phi}$	Electric potential		
$\hat{L}$	Lagrangian	$\hat{H}$	Hamiltonian
$\hat{W}$	Work	$\hat{P}$	Power
L	Effective Lagrangian	H	Effective Hamiltonian
η	Acoustofluidic yield	α	Acoustophoretic mean orientation

2. Theory

The free Lagrangian densities, i.e. with no boundary contributions, for a system constituted by an elastic solid, an inviscid fluid, and a piezoelectric element driven at a given frequency in an oscillatory regime are

$$\mathscr{L}_{\mathrm{m}}(\boldsymbol{u}, \boldsymbol{\nabla}\boldsymbol{u}) = \rho\omega^2 \boldsymbol{u}^* \cdot \boldsymbol{u} - \boldsymbol{\nabla}\boldsymbol{u}^* : \boldsymbol{\Sigma} : \boldsymbol{\nabla}\boldsymbol{u}, \tag{1}$$

$$\mathscr{L}_{\mathrm{a}}(p, \boldsymbol{\nabla}p) = \frac{\boldsymbol{\nabla}p^* \cdot \boldsymbol{\nabla}p}{\rho\omega^2} - \frac{p^* p}{\rho c^2}, \tag{2}$$

$$\mathscr{L}_{\mathrm{em}}(\boldsymbol{u}, \boldsymbol{\nabla}\boldsymbol{u}, \phi, \boldsymbol{\nabla}\phi) = \rho\,\omega^2 \boldsymbol{u}^* \cdot \boldsymbol{u} - \boldsymbol{\nabla}\boldsymbol{u}^* : \boldsymbol{\Sigma} : \boldsymbol{\nabla}\boldsymbol{u} + \boldsymbol{\nabla}\phi^* \cdot \boldsymbol{\varepsilon} \cdot \boldsymbol{\nabla}\phi - 2\,\boldsymbol{\nabla}\phi^* \cdot \boldsymbol{P} : \boldsymbol{\nabla}\boldsymbol{u}\,. \tag{3}$$

The meaning of the symbols appearing in these equations is given in table 1. We note that for the system we are considering, the field variables, i.e. the displacement, the pressure and the electric potential, should be labeled to address which subsystem of the device, they refer to. For the sake of clarity we omit this index to better illustrate the general idea of the variational framework. Thus, the corresponding Euler–Lagrange equations for the system of equations (1)–(3) that govern the behavior of the system in the oscillatory regime with angular frequency ω, can be retrieved by varying the Lagrangian densities with respect to the field variables $\boldsymbol{u}$, p, and ϕ. When we want to implement the governing equations in a finite element software, such as Comsol Multiphysics, we need just to provide the Lagrangian densities (1)–(3) and the boundary contributions to these. The latter are given by

$$\mathscr{L}_{\mathrm{m}}^{\mathrm{bnd}}(\boldsymbol{u}, \boldsymbol{\sigma}_{\mathrm{m}}^{\mathrm{bnd}}) = \boldsymbol{u}^* \cdot \boldsymbol{\sigma}_{\mathrm{m}}^{\mathrm{bnd}} \cdot \hat{\boldsymbol{n}}, \tag{4}$$