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MODELING, SIMULATION, AND OPTIMIZATION OF SURFACE ACOUSTIC WAVE DRIVEN MICROFLUIDIC BIOCHIPS*

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Abstract

We will be concerned with the mathematical modeling, numerical simulation, and shape optimization of microfluidic biochips that are used for various biomedical applications. A particular feature is that the fluid flow in the fluidic network on top of the biochips is induced by surface acoustic waves generated by interdigital transducers. We are thus faced with a multiphysics problem that will be modeled by coupling the equations of piezoelectricity with the compressible Navier-Stokes equations. Moreover, the fluid flow exhibits a multiscale character that will be taken care of by a homogenization approach. We will discuss and analyze the mathematical models and deal with their numerical solution by space-time discretizations featuring appropriate finite element approximations with respect to hierarchies of simplicial triangulations of the underlying computational domains. Simulation results will be given for the propagation of the surface acoustic waves on top of the piezoelectric substrate and for the induced fluid flow in the microchannels of the fluidic network. The performance of the operational behavior of the biochips can be significantly improved by shape optimization. In particular, for such purposes we present a multilevel interior point method relying on a predictor-corrector strategy with an adaptive choice of the continuation steplength along the barrier path. As a specific example, we will consider the shape optimization of pressure driven capillary barriers between microchannels and reservoirs.

Mathematics subject classification: 49K20,49M37, 65K10, 65M60, 65N30, 76N10, 76Z05, 78A70, 90C30, 92C35.
Key words: Microfluidic biochips, Mathematical modeling, Numerical simulation, Shape optimization, Multiphysics, Multiscale problems.

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1. Introduction

Microfluidic biochips are used in pharmaceutical, medical, and forensic applications for high throughput screening, genotyping, and sequencing in genomics, protein profiling in proteomics, and cytometry in cell analysis [19, 43, 46, 51]. They provide a much better sensitivity and a greater flexibility than traditional approaches and, most importantly, give rise to a significant speed-up of the hybridization processes. This can be achieved by integrating the fluidics on top the chip by means of a lithographically produced network of channels and reservoirs (cf. Fig. 1.1 (left)).

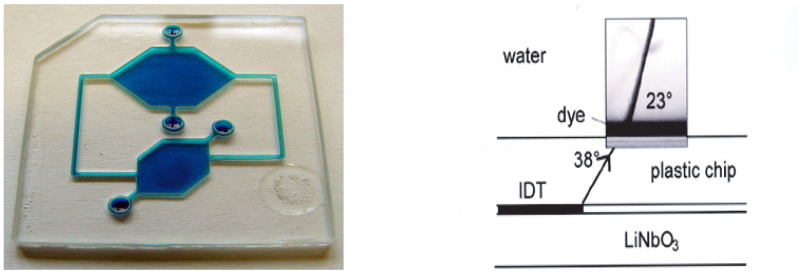

Fig. 1.1. Microfluidic biochip (left) and sharp jet created by surface acoustic waves (right)

The idea is to inject a DNA or protein containing probe and to transport it in the fluid to a reservoir where a chemical analysis is performed. The fluid flow can be taken care of by external pumps which, however, are subject to wear. Instead, a new generation of biochips is based on a surface acoustic waves (SAW) driven fluid flow [25, 53, 54]. Surface acoustic waves are generated by interdigital transducers (IDT), propagate through the base of the device with amplitudes in the range of nanometers and enter the fluid filled microchannels thus creating a sharp jet (cf. Fig. 1.1 (right)). This happens within nanoseconds. The SAWs experience a significant damping along the microchannels which results in a stationary flow pattern, called acoustic streaming. This relaxation process occurs on a time-scale of milliseconds. We are thus faced with a multiscale, multiphysics problem whose mathematical modeling and numerical simulation represents a significant challenge. It is also a challenging problem with regard to various optimization issues such as the optimal design of the microchannels in order to achieve a maximum pumping rate. Another one is the design of pressure driven capillary barriers between the channels and the reservoirs to guarantee a precise filling of the reservoirs with the probes (cf. Fig. 1.2). This amounts to the solution of a shape optimization problem where the mathematical model for the acoustic streaming represents the associated state equations.

The paper is organized as follows: In section 2, we will present a mathematical model for

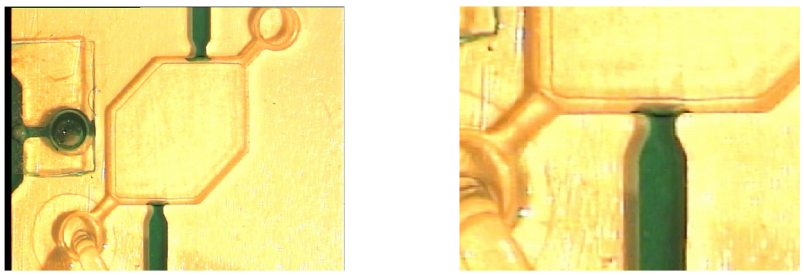

Fig. 1.2. Capillary barriers