Modeling, Simulation and Optimization of Surface Acoustic Wave Driven Microfluidic Biochips

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Abstract

Biochips are physically and/or electronically controllable miniaturized labs. They are used for combinatorial chemical and biological analysis in environmental and medical studies, e.g., for high throughput screening, hybridization and sequencing in genomics, protein profiling in proteomics, and cytometry in cell analysis. The precise positioning of the samples (e.g., DNA or proteins) on the surface of the chip in picoliter to nanoliter volumes can be done either by means of external forces (active devices) or by specific geometric patterns (passive devices). The active devices which will be considered here are microfluidic biochips where the core of the technology are nanopumps featuring surface acoustic waves generated by electric pulses of high frequency. These waves propagate like a miniaturized earthquake (nanoscale earthquake), enter the fluid filled channels on top of the chip and cause an acoustic streaming in the fluid which provides the transport of the samples. The mathematical model represents a multiphysics problem consisting of the piezoelectric equations coupled with multiscale compressible Navier-Stokes equations that have to be treated by an appropriate homogenization. We discuss the modeling approach, present algorithmic tools for the numerical simulation and address optimal design issues as well. In particular, the optimal design of specific parts of the biochips leads to large-scale optimization problems. In order to reduce the computational complexity, we present a combination of domain decomposition and balanced truncation model reduction which allows explicit error bounds for the error between the reduced order and the fine-scale optimization problem. It is shown that this approach gives rise to a significant reduction of the problem size while maintaining the accuracy of the approximation.
The results are based on joint work with Harbir Antil, Roland Glowinski, Matthias Heinkenschloss, Daniel Köster, Christopher Linsenmann, Kunibert Siebert, Danny Sorensen, Tsorng-Whay Pan, and Achim Wixforth.