Multiscale Modeling of Microfluidics

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Micro-electro-mechanical systems involve complex functions governed by diverse transient physical and electrical processes for each of their many components. A generic example of a largely simplified microfluidic system is shown schematically in figure 1. This system is made up of a micropump, a flow sensor, and an electronic control circuit. The electronic circuit may be used to adjust the pump flow rate so that a constant flow is maintained in a microchannel. The simulation of the complete system requires models for the micropump, the microflow sensor, and the electronic components associated with the control circuit. This is an example of a *coupled-domain simulation*, i.e., the simultaneous simulation of different functional units of the device. In coupled-domain problems, such as flow-structure, structure-electric or a combination of both, there are significant *disparities* in temporal and spatial scales. This, in turn, implies that multiple grids and heterogeneous time-stepping algorithms may be needed for discretization, leading to very complicated and consequently computationally prohibitive simulation algorithms. Simplifications are typically made with one of the fields represented

- At reduced resolution level, or
- By low-dimensional systems, or
- By equivalent lumped dynamical models.

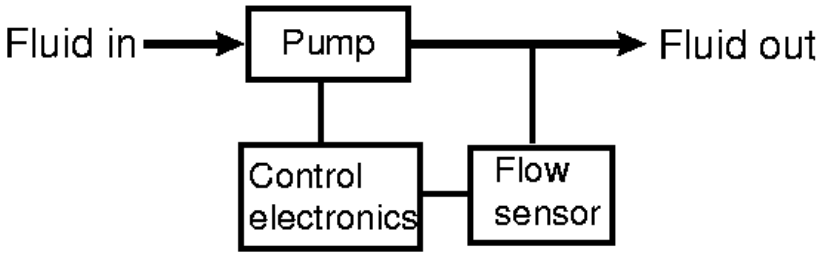

Figure 1: Block diagram of a generic microfluidic system. The flow sensor senses the flow rate which is controlled by the electronic circuit controlling the pump.

The design-complexity and functionality-complexity of MEMS exceed by far the complexity of VLSI systems. However, three decades ago VLSI simulation was considered a formidable task but

today VLSI systems are simulated routinely thanks to the many advances in CAD and simulation tools achieved over that period. It is clear that similar and even greater advances are required in the MEMS field in order to make *full-system simulation* of MEMS a reality in the near future. This will enable the MEMS community to explore new pathways of discovery and expand the role and influence of MEMS at a rapid rate. In order to develop such a system-level simulation framework, which is sufficiently simple, accurate and robust, *all processes* involved need to be simulated at a comparable degree of accuracy and integrated seamlessly. That is, circuits, semi-conductors, springs and masses, beams and membranes, as well as the flow field need to be simulated in a consistent and compatible way and in reasonable computational time! MEMS simulation based on full-physics models is more appropriate for exploring new concepts whereas macromodeling may be employed effectively for familiar designs and in known operating regimes.

The main disadvantage of a full-system simulation approach is the high computational cost involved. The principal cost comes from solving the three-dimensional time-dependent flow equations in complex geometric domains, in transition regimes and with unfamiliar physics. It is, therefore, important to obtain a fundamental understanding of microflows, first in order to construct low-dimensional models similar to what has been done in flows at large scales, and second to explore new design concepts based on new physics.

The main differences between fluid mechanics at microscales and in macro domain can be broadly classified into four areas:

- Non-continuum effects,
- Surface-dominated effects,
- Low Reynolds number effects, and
- Multi scale and multi physics effects.

Some of these effects can be simulated with relatively simple modifications of the standard simulation procedures of computational fluid dynamics. However, others require new simulation approaches not used in the macrodomain. For gas microflows, compressibility effects are very important because of relatively large density gradients, although the Mach number is typically low. Depending on the degree of rarefaction, corrections at the boundary or everywhere in the domain need to be incorporated. Increased rarefaction effects may make the constitutive models for the stress tensor and the heat flux vector in the Navier-Stokes equations invalid. On the other hand, working with the Boltzmann equation or with molecular dynamics implementation of Newton's law directly is computationally prohibitive for complex micro geometries. The same is true for liquids as atomistic simulation based on Newton's law for individual atoms is restricted to extremely small volumes. Therefore, hybrid atomistic-continuum methods need to be employed for both gas and liquid microflows to deal effectively with deviations from the continuum and to provide a link with the large domain sizes.

In this lecture, we will discuss *gas*, *liquid*, and *particulate* microflows and present governing equations, simplified models, and efficient numerical methods that can be used in simulations. Because of the unfamiliar physics involved, detailed simulations are required and this necessitates either using atomistic (particle-based) simulations or adding correction terms to the macroscopic full simulation methods. For example, in the slip flow regime it is reasonable to employ the Navier-Stokes equations modified at the wall surface with appropriate velocity slip and temperature jump conditions.

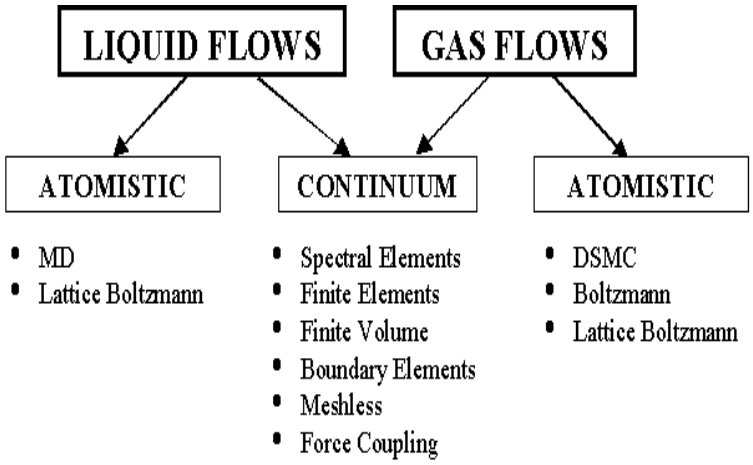

Figure 2: Summary of simulation methods for liquid and gas microflows.

In the first part we present simulation results and macromodels for gases. We use both continuum-based modified spectral element simulations [1] as well as Direct Simulation Monte Carlo (DSMC) and Boltzmann solutions to investigate slip flow and transition regimes for microducts and separated prototype flows. A general slip model is proposed that is robust and easy to use in continuum-based simulations. We then review simulation advances in liquid flows with specific emphasis on electroosmosis and flow control [2]. High resolution simulations are presented (performed by A. Beskok and his students) that resolve the Debye layer region. A new bounday condition is proposed that is suitable for mixed electroosmotic/pressure-driven flows and validated with results from full simulations. Finally, we adress issues in bio-particulate flows and introduce the Force Coupling Method (FCM) that represents efficiently motion of particles in microflows. This method, which was developed by Maxey and collaborators, is based on multipole expansions that represent the action of virtual particles and thus no special meshes or re-meshing is required during the computation. A comparison with experimental results will be presented that shows good aggreement for the trajectories and velocities of multiple particles.

In closing, we will summarize the potentially most effective numerical methods in microfluidic simulations (including meshless methods, Lattice Boltzmann methods, and stochastic approaches) and discuss their relative advantages.

References

- G.E. Karniadakis and S.J. Sherwin, *Spectral/hp Element Methods for CFD*, Oxford University Press, 1999.
- G.E. Karniadakis and A. Beskok, *Microflows: Fundamentals and Simulation*, Springer, 2001.