Computational Mechanics in MEMS: From Spanning the Scales to Order Reduction

Jan G. Korvink, Andreas Greiner and Evgenii B. Rudnyi

IMTEK – Institute for Microsystem Technology
Faculty for Applied Science
Albert Ludwig University Freiburg
Georges-Koehler-Allee 102, 79110 Freiburg, GERMANY
korvink@imtek.de

Computational mechanics for micro-electro-mechanical systems (MEMS) is faced with a fundamental dilemma. Device feature sizes often lie at the limit regime where the continuum description is no longer sufficient. This means that to get more accurate, we have to move to increasingly molecular-based models. For a reasonable chunk of material, this drastically increases the size of a simulation, and the time to solve the resulting equations of motion. One strategy to obtain reasonably sized models that capture enough detail is the so-called multiscale approach. This relies on a deep understanding of the underlying physical principles and a prudent mix of differently resolved models. Another strategy is to take the large equations of motion that arise, and to mathematically reduce their order before solving.

The coarse graining of Molecular Dynamics (MD) is a first step towards multiscale modeling and simulation. The most promising candidate to accomplish this goal is Dissipative Particle Dynamics (DPD). It provides a substantial reduction in the number of degrees of freedom compared to MD. The coupling to continuum simulations can improve the efficiency even more. Apart from particle-based models there are the Lattice Boltzmann (LB) approaches, dealing with the equation of motion of a single particle distribution function as represented by the Boltzmann transport equation. The application of either LB or DPD depends very much on the requirements of the simulation. In the first case higher moments of the distribution function are calculated, in the second case inhomogeneities, phase transitions, and multicomponent systems are described. For both models the missing link to continuum approaches up to a systems description is still an open field of research.

A major computational challenge is the integration of nonlinear ordinary differential equations in time. In many cases one can find a low-dimentional equivalent that approximates the original high-dimensional system with good accuracy. Compact modeling enjoys widespread use in the engineering community for quite some time. Compact modeling is based on engineering intuition and it is quite difficult to employ for arbitrary devices. Modern mathematics suggests a competitive approach to model order reduction, where the low-dimensional approximation can be found automatically by means of formal algorithms. Here, model reduction is compact modeling on demand. Model reduction is a dynamic scientific area and we believe that in the near future it will play a substantial role in simulation.

Clearly, a clever combination of the latest achievements in hardware, algorithms and modeling will allow us to create realistic but fast computer models also for mesoscale devices.

References

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