Modeling Strategies for Microsystems

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Abstract

A hierarchical approach to microsystem modeling is outlined. On the device level, the operating behavior is analyzed on the basis of continuous field models. To deal with the coupling effects typical of microsystems, various coupling schemes between single-effect simulators can be used. Equipped with the direct insight into the device operation, compact models are developed. Starting from a thermodynamic system description, the reduction to only a small number of degrees of freedom leads to compact models, which still correctly reproduce the relevant conservation laws and, therefore, can be connected to form a Generalized Kirchhoffian Network. This is equivalent to a system of ordinary algebro-differential equations for the node variables, which is solved using one of the standard analog network simulators available. As an illustrating example, the analysis of an electrostatically driven micropump is presented. Starting from a detailed analysis of the constituent parts of the pump, a system macromodel is set up and utilized for analyzing a typical operation regime.

Keywords: Microsystem compact models; Kirchhoffian Networks; Coupled Fluid–Structure FEM; Micropump

Motivation

In the recent years, microsystems technology has made rapid progress in the realization of miniaturized 'smart' components with complex functionality, which yet remain amenable to cost-effective fabrication and reliable operation. Various products reached the stage of mass production by the use of industrial semiconductor technology. So the scene is ready to bringing many novel ideas and concepts as new products to the marketplace. One prerequisite for the further success of this development is the availability of a set of efficient design tools, which fit in with today's far advanced design environments used in the semiconductor industry and, in particular, are conform with the widely accepted bottom-up and top-down modeling hierarchies.

It is an inherent problem of microsystem modeling, that most of the constituent components, by their function as transducer elements, couple different physical energy and signal domains. As a consequence, the models underlying the simulation tools must be capable of accounting for a large variety of physical coupling effects.

In this work, we will briefly analyze the present situation in the field, leading us to a modeling strategy from continuous field models (CFM) on the device level up to compact models (CM) for system simulation. After exemplifying the approach in the light of a microfluidic system (micropump), we will derive some demands seeming most relevant to the future development.

Continuous Field Models for Coupled Problems

The natural description of the physical operation of coupled transducer elements is provided by continuum models which couple the relevant field quantities (mechanical, thermal, electric, magnetic,...) consistently in terms of a (typically quite complex) system of partial differential equations. There are two basic coupling mechanisms: coupling by volume (e.g. piezoelectricity or thermoelasticity) and coupling through the common interface of adjacent system domains (e.g. electrostatic or pressure forces on diaphragms). Volume-coupled problems can sometimes be solved directly by means of FEM provided that problem-specific coupled-field elements have been implemented. For surface-coupled problems, efficient global solution methods based on partitioning and domain decomposition are available, but rarely implemented in existing simulation environments. Very often we find commercial device simulators adapted to one of the single physical effects, suggesting the use of iterative interfacing techniques for the external coupling of the existing tools.

Basically four approaches have proven to be successful. In the semianalytical approach, one or more of the coupled parts of a device are described by simplified analytical models which interact through interface conditions with the other coupled parts described by FEM models. The overall accuracy of this method strongly depends on the idealizations made, restricting it to simple geometries and material laws.

In the second approach, existing simulators calculate in their specific space and energy domain(s) and communicate with each other along the connecting interfaces according to an iterative scheme (typically a relaxation algorithm, see Fig. 1). This method is restricted mostly to small deviations from equilibrium and usually lacks convergence under strong coupling conditions [1].

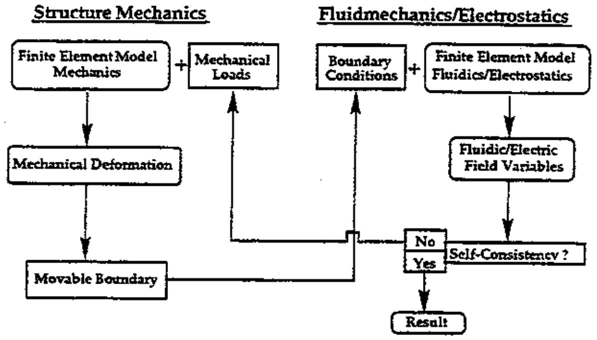

Figure 1: Iterative solution approach for fluid-structure interaction and surface-coupled electromechanical problems.

The third approach avoids those convergence problems by the simultaneous solution of all governing equations using special, problem-specific numerical methods (e.g., domain decomposition, non-conforming grids etc.). However, this approach cannot be based on available commercial tools and, hence, requires new software implementations. In addition, the computational expense may easily exceed the hardware limitations.

Hence, to avoid this drawback while sustaining numerical stability and speed, the relaxation scheme of the second approach is replaced by a Newton iteration, where the required Jacobians are set up only by calls of the single effect simulators. Therefore, no code modifications are necessary [2], [3].

However, all the four above-mentioned approaches will fail in the vicinity of an unstable operating point (e.g., snap back effect). In this situation, homotopy methods are useful to tackle the problem. Here, an appropriate homotopy parameter is introduced which allows to externally control the state variables. Starting with a parameter value where the solution is easy to be computed, the desired operating point is attained by path continuation [4]. This algorithm may be employed as exterior loop in any of the approaches described before.

Generalized Kirchhoffian Networks

Considering the numerical effort required for realistic microdevices and systems, the use of continuous field models (CFM) becomes easily prohibitive. Therefore, the number of degrees of freedom has to be reduced to an amount that is still manageable and yet accurate enough for predictive simulation. A proper approach is analog circuit simulation based on compact models (CM) of the constituent microsystem components derived from the CFMs and a network theory which preserves the basic conservation laws expressed in the CFMs.

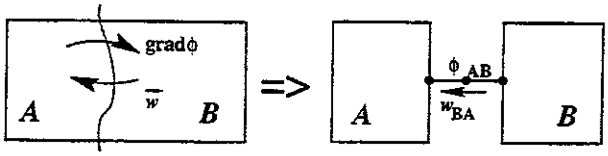

Figure 2: A system is partitioned into blocks by defining an appropriate interface (left) and lumping the exchange of flux quantities into single nodes (right).

A systematic way to develop CMs is, among others, provided by a thermodynamic system description in terms of driving forces and resulting fluxes of the relevant physical quantities [5]. Partitioning the system into blocks and lumping the exchange of flux quantities between adjacent subsystems along common interfaces into single nodes (Fig. 2) eventually yields a full system description as "Generalized Kirchhoffian Network", which is governed by generalized mesh rules and node rules expressing the basic conservation laws for energy, mass, charge etc. This is equivalent to a system of ordinary algebro-differential equations for the node variables, which can be solved using a standard analog network simulator. The network parameters may either be extracted from measurements or from numerical CFM simulations. Since the CM equations are derived from physical CFMs, all state variables and nearly all model parameters represent physical quantities or geometrical or material data. Therefore, the model parametrization can be based mostly on technological and material data instead of intransparent and device-dependent curve fittings.

A generic software approach to CM is a hardware description language like VHDL-AMS [6], which constitutes a standardized model interface in analog network simulators and, furthermore, allows the description of arbitrary physical energy and signal domains in addition to the electrical quantities.

Dynamic Micropump Macromodel

As an illustrative example, we refer to a microfluidic system with integrated control electronics and demonstrate the simulation of an electrostatically actuated micropump as developed by R. Zengerle [7]. It consists of a pump chamber with an electrostatically actuated membrane as the driving element, inlet and outlet passive check valves and external connection tubes (Fig. 3).

The analysis of the complex transient behavior of the micropump requires a detailed understanding of the

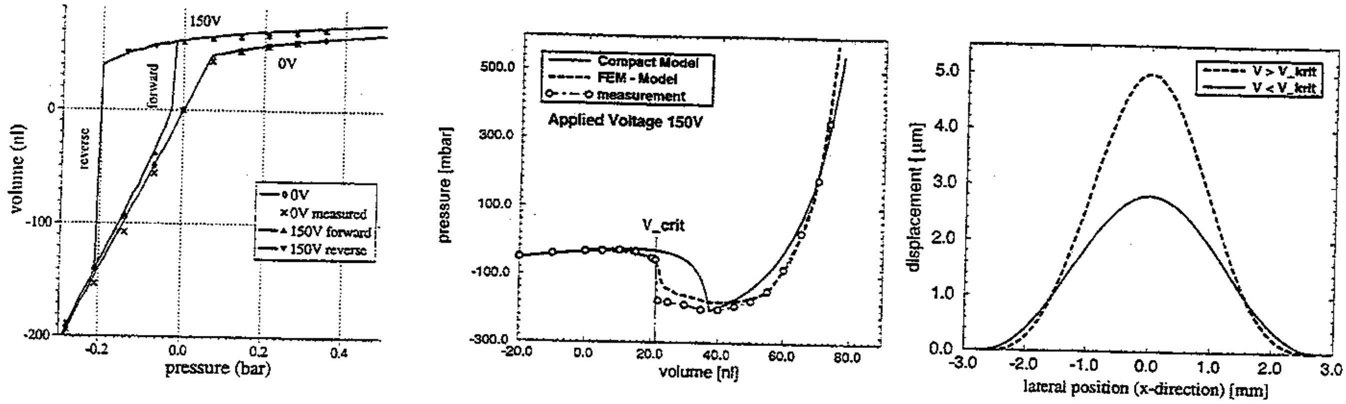

Figure 4: Static characteristics of a membrane as a function of the pressure in the pump chamber (left) and as a function of the externally enforced fluid volume (middle). Shape snapping of the membrane (right) occurs, when a critical volume is forced into the pump chamber.

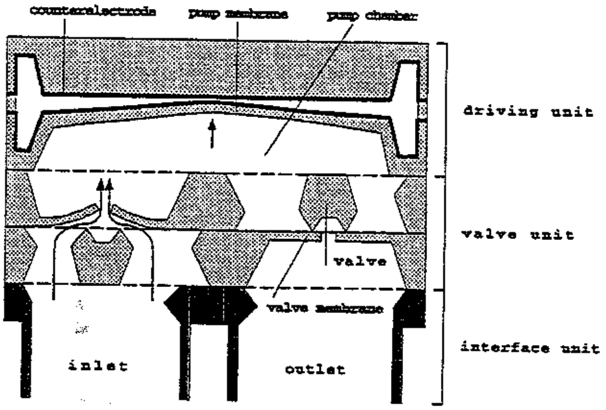

Figure 3: Schematic view of a micropump, consisting of an electrostatically actuated membrane attached to the voltage supply circuitry, the valves and the connecting tubes.

operation of the constituent parts on the basis of CFM. Both the membrane and the flap valve exhibit strong coupling between different physical domains. Therefore, the electro-mechanical coupling determining the membrane behavior as well as the fluid structure interaction between fluid and valve flap are modeled using two commercial FEM tools coupled through a relaxation scheme (Fig. 1). The resulting static membrane characteristics as a function of the pressure in the pump chamber and as a function of a forced fluid volume in the pump chamber are presented in Fig. 4, illustrating characteristic effects of electrostatically actuated membranes such as the hysteresis of the snap-down effect and the shape snapping. From these results a compact model was derived, which describes the membrane behavior by a single state variable, but is, due to the snap-down of the membrane, discontinuous in nature. Comparisons between CM and CFM simulations show that important phenomena of the membrane behavior like hysteresis and snap-down can be accurately modeled by the compact model. To model the shape snapping of the membrane occurring at the snap-down point, additional state variables would be required. To keep the membrane model as simple as possible, we decided to neglect this effect. Therefore, the static membrane behavior for forced volume flow into the pump chamber cannot be reproduced exactly by the CM in the snap-point region (Fig. 4). For the macromodel of the entire micropump, however, this effect turns out to be of minor relevance and, thus, may be neglected in the CM of the membrane.

From the static flow rate and the pressure-dependent nonlinear displacement of a passive check flap as obtained by CFM simulations, a CM is derived which describes the deflection of the entire valve by a single state variable. The comparison between CM and CFM results as well as to measured data from [8] reveals very good agreement (Fig. 5). Transient CFM simulations enable us to extract the eigenfrequency and the damping parameters for the oscillating valve flap in the fluid (Fig. 6). Turbulent effects occurring in the fluid around the flap (Fig. 7) result in a nonlinear damping behavior. Combining the extracted parameters from CFM simulations of both the transient and static behavior leads to a CM which reproduces the static as well as the dynamic valve behavior in a sufficiently accurate way.

The compact models of the valves and the electrostatically actuated membrane are then combined with the model for the tubes as described in [9], resulting in a macromodel for the entire micropump including the electric control circuit (Fig.8).

The pump rate is investigated as a function of the driving frequency. The effect of reverse pumping as reported in [7] can be correctly reproduced, and the evidence of nonlinear damping terms in the valve CM on the dynamic behavior of the pump is illustrated in Fig. 9. The results shown in Fig. 10 give rise to the assumption that both valve flaps together with the fluid in the pump chamber act as a coupled oscillator system. To analyze

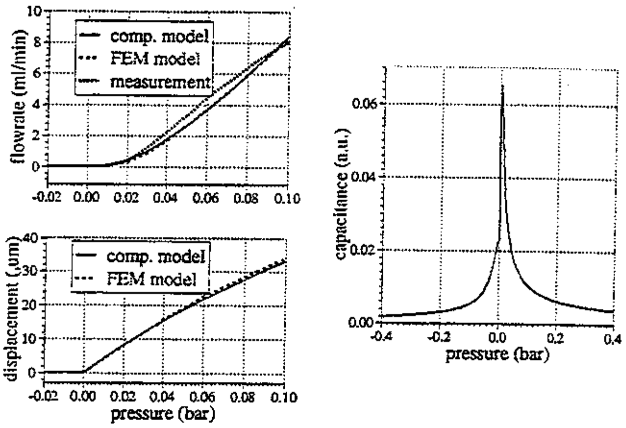

Figure 5: Static characteristics of a valve: flap displacement, mass flow rate and fluidic capacitance versus applied pressure.

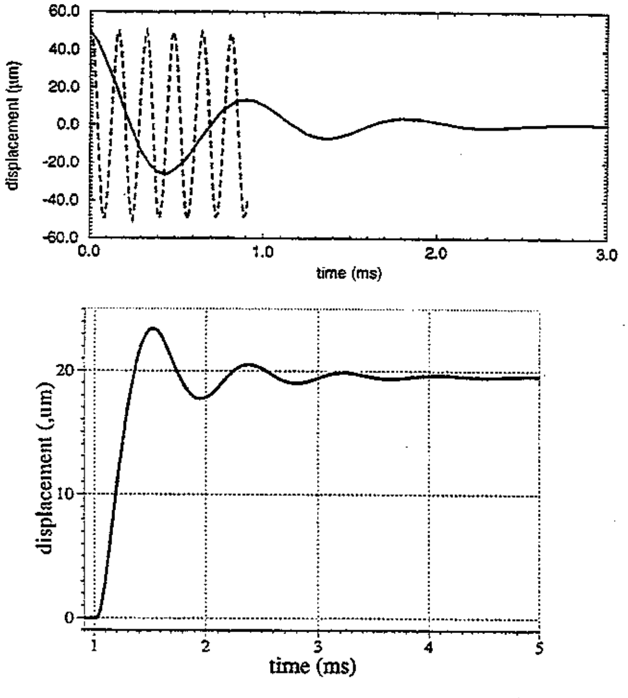

Figure 6: Top: FEM simulation of the transient behavior of a valve flap without (dotted line) and with (solid line) damping caused by the surrounding liquid. The flap is initially displaced by $50\mu m$ and then released to oscillation. In presence of the liquid, the oscillation frequency decreases and strong damping is observed. Bottom: Simulated flow rate and flap displacement of a valve as caused by a steplike pressure change from reverse to forward direction.

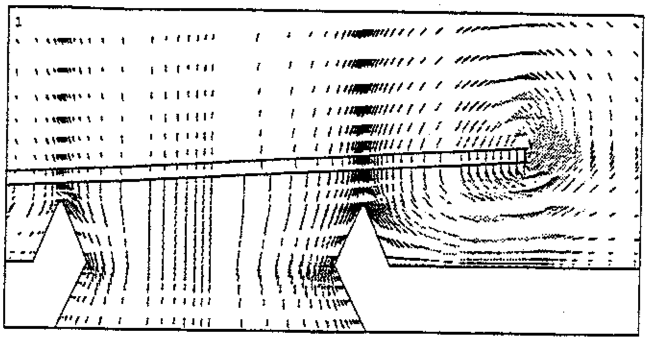

Figure 7: Transient FEM simulation of the fluid velocity in a valve chamber with an oscillating valve flap. The velocity ranges from 0 to 1m/s. The vertical dimensions of the valve are stretched by a factor of 2.

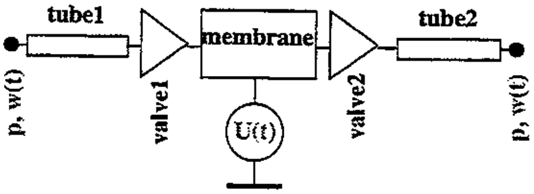

Figure 8: Macromodel of the entire micropump as a Generalized Kirchhoffian Network of the compact models of all constituent parts of the micropump.

the details of this coupled oscillation a reinvestigation by means of CFM simulations would be necessary. It is worthwhile to note that the full system simulations lend us insight in details of the involved interaction of the system parts which would not have been revealed by means of CFM due to the complexity of the problem.

Future Perspectives

We discussed modeling strategies for CFM and CM as the essential parts of a comprehensive methodology of bottom-up and top-down microsystem modeling and demonstrated the efficiency of our hierarchical approach considering an electro-microfluidic system as illustrative example. Now efforts must be made to transform these results in robust, easy-to-use software packages which are ready for the use in existing CAD environments. This implies that, on the CFM level, software tools must be developed which allow for the efficient interfacing of different single-effect simulators in such a way that new advanced coupling schemes can be realized by a flexible control of the solution process.

On the system level, libraries of CMs have to be established, preferably in a simulator-independent generic hardware description language such as VHDL-AMS. In addition, parameter extraction and model validation techniques for CMs, using CFM simulation results as

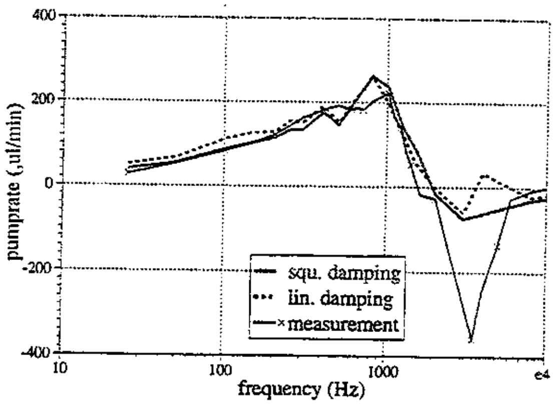

Figure 9: Simulated pump rate vs. driving frequency. The damping of the valve flap is modeled as a linear function of the flap velocity (dotted line), and also with quadratic terms included (solid line).

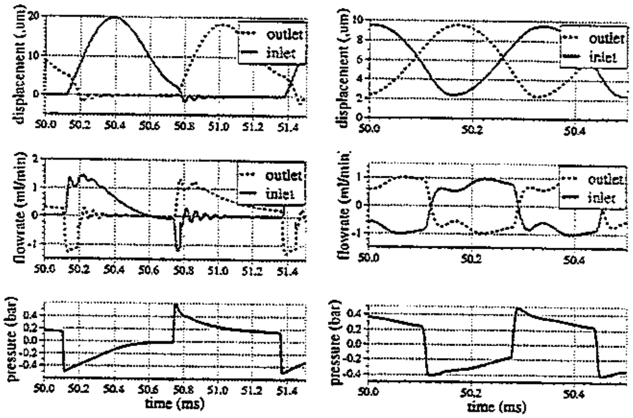

Figure 10: Transient simulated flap displacement and flow rate at inlet and outlet valve and mean pressure in the pump chamber. The pump is operated near the fundamental resonance frequency of the valve flap (left) or above the resonance frequency (right). A single pump cycle is shown in both cases.

well as measured data, are required. The corresponding software tools are the indispensable prerequisite for statistical modeling, which again addresses such important topics as fabrication yield and reliability.

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