1-3 (Plenary)

Coupled-Field Modeling of Microdevices and Microsystems

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Abstract – **Currently strong efforts are being made to build simulation platforms for the predictive simulation of microelectromechanical devices and microsystems (MEMS) as cost-effective and time-saving alternative to the traditional experimental approach. Already today the rapid progress in microsystems technology is strongly supported by MEMS-specific modeling methodologies and dedicated simulation tools constituting a "virtual laboratory" on the computer, which enables the visualization and detailed analysis of the operating behavior of single microdevices as well as their collaborative function in a microsystem. In this context, one of the most important aspects is the consistent treatment of coupled fields and coupled energy and signal domains required for deriving macromodels of microsystems from the continuous field level. To this end, we discuss practicable methodologies for setting up physically-based consistent microdevice and full system models for the effort-economizing and yet accurate numerical simulation of micromechatronical components and systems.**

1. Motivation

The potential offered by microsystems technology makes it possible to satisfy progressively challenging user demands by realizing products which are "intelligent" in the sense that they exhibit an integrated self-learning and self-controlling multi-functionality. Currently we find a rapid progress in the manufacturing of miniaturized "smart" components with complex functionality, which yet remain amenable to cost-effective fabrication and reliable operation.

In the development of such "smart" microsystems we face the problem that intricate trade-off considerations govern the layout and design as well as the operating conditions of microsystems and their constituent components. Therefore a systematic improvement of the performance is hardly possible without being equipped with a profound expertise in the details of the operating behavior of single microsensor or actuator elements and their interaction in complete microsystems with co-integrated or hybrid coupled electronic circuitry for power supply, signal conditioning, and system control including (self-)test and (self-)calibration as well as error detection and compensation.

Using numerical simulation, the required expertise can be gained faster and cheaper than by experimental investigations. Hence, modeling and numerical simulation is widely accepted as cost-effective and time-saving alternative to the traditional experimental approach by "straightforward trial and error".

Evidently it is an inherent problem of microsystem modeling that most of the constituent components, by their nature as transducer elements, couple different energy and signal domains such as mechanical, fluidic, thermal, electrical, and other physical or chemical quantities (Fig. 1). As a consequence, the models underlying the simulation tools must be capable of accounting for a large variety of physical coupling effects on the device level as well as on the system level. Here, we face two tasks: Developing practical methods for setting up easy-to-use problem-specific models on the respective descriptive level (device or system), and implementing these models in a set of efficient simulation 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.

2. Specific Aspects of MEMS Modeling

As the state of the art in modeling, simulation, and design optimization is far advanced in the world of microelectronics, it seems attractive to adopt the well-tried methodologies and tools for model generation and parameter extraction used in the IC world and to use them also in the field of MEMS. However, in spite of what they have in common, there are several aspects in which microsystems technology largely differs from integrated circuit (IC) technology. Integrated circuits are composed of a quite limited number of elementary device structures (such as MOSFETs and capacitor cells), fabricated by means of well-established and quasi-standardized design rules and process technologies. In the field of MEMS technology, on the other hand, an ever growing variety of different device types has emerged, based on rather unconventional design methods and a large number of widely differing (and sometimes very unconventional) fabrication technologies. Therefore, today's challenge in the computer-aided IC design consists in mastering very complex system topologies built up by a huge number of simple basic elements, whereas in the computer-aided design of microelectromechanical systems we face the problem of describing systems with simple topology built up by a comparably small number of constituent components which, however, exhibit a high functional complexity based on quite sophisticated and involved physical operating principles.

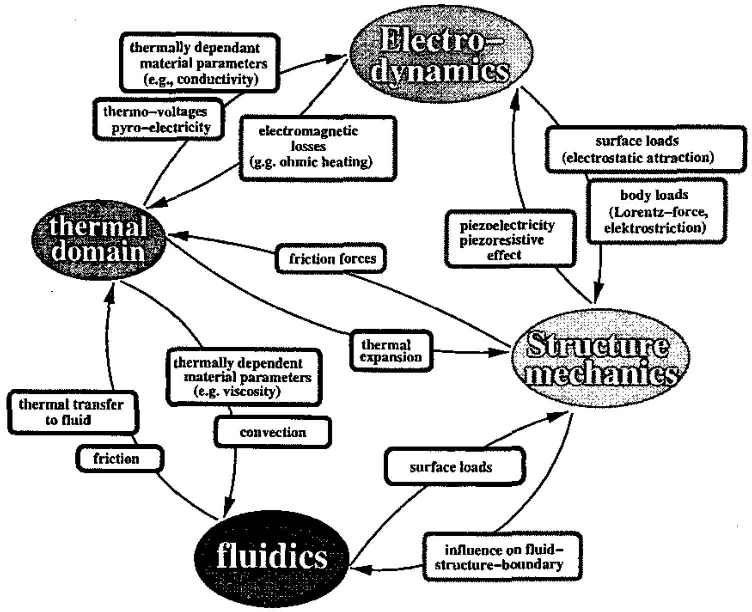

Fig.1: Physical coupling effects arising in micromechatronical devices and systems.

The complexity of microsystems originates in particular from the afore-mentioned complicated coupling effects between different energy and signal domains (Fig. 1) which, on the one hand, is the inherent and much desired property of any sensor and actuator element in a microsystem and, on the other hand, is a detrimental property when it occurs as parasitic cross-coupling between the system components. Hence the accurate analysis of all kinds of physical coupling effects has a major impact on the optimization of microsystems and is thus the most important issue that has to be tackled in the computer-aided design of microdevices and microsystems. In this sense, the physically-based, but yet computationally tractable modeling of microsystems is widely recognized as necessity and challenge, even though it may easily become quite involved and computationally expensive. Therefore the computational effort as well as the time spent into model development, validation, calibration, and parameter extraction have to be carefully adjusted with respect to the actual needs, as it has been proposed by the concept of "tailored modeling" [1].

To this end, the methodological approaches and analysis tools used in IC modeling need to be modified in order to properly account for the particular demands on the models arising from their dedicated application to MEMS. Implementation in a "CAD toolbox for MEMS", similar to the well-established TCAD frameworks in the IC world, will then allow for an efficient and time-economizing computer-aided microsystem development. First commercial MEMS simulation platforms are already available [2-8] and appear quite promising, even though their application is still restricted with respect to the geometric and functional complexity and the included coupling effects on device and system level.

3. Continuous-Field Multi-Physics Models of Microdevices

The natural and most rigorous, but also most expensive description of the physical operation of single microdevices as well as their interplay as constituent elements in a microsystem is provided by continuous-field models (CFM) which couple the relevant field quantities (mechanical, thermal, electric, magnetic, optical, chemical..., see Fig. 2) consistently in terms of a (typically highly non-linear) system of partial differential equations. Very often these equations have the common generic structure of balance equations:

$$\frac{\partial n_X}{\partial t} + \vec{\nabla}\vec{J}_X = \Pi_X \qquad (1)$$

where n_X, J_X *and* P_X denote the density, the current density and the production rate of an extensive field variable $X(r,t)$. The current densities obey the constituent pseudo-linear current relations

$$\vec{J}_X = -\sum_Y L_{XY}\vec{\nabla}\phi_Y \qquad (2)$$

where the potentials $\Phi_Y(r,t)$ play the role of driving forces for the fluxes $J_X(r,t)$ and the (state-dependent) transport coefficients L_{XY} represent (one class of) coupling effects between different energy domains. One should note that it is this generic structure of the continuum models which provides the natural link to a system level description in terms of Kirchhoffian network theory (see sec. 4.2).

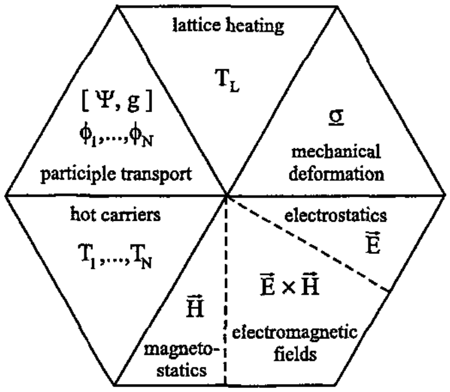

Fig.2: Coupled energy domains and continuous field variables used for MEMS device modeling.

On the continuous field level, after selecting the proper physical models and state variables and defining the external operating conditions and control parameters (such as applied pressure or mechanical stress, ambient temperature, bias voltages, magnetic fields etc.), the internal operating behavior is studied by numerical solution of the underlying dynamical equations. Depending on the problem considered, the numerical studies may include stationary or transient mechanical structure analysis, electrostatic or magnetostatic analysis, thermal analysis, fluid and gas transport analysis, electronic transport analysis, and all possible combinations thereof (coupled-field analysis). This simulation level is most important for the optimization of the individual system components.

The transducer and parasitic coupling effects appear as a result of the self-consistent solution of the coupled system of dynamical equations linking the different physical energy and signal domains. There are two basic coupling mechanisms: coupling by volume (e.g. piezoresistivity 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 the Finite Element Method (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 frameworks. 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.

From the various solution methods which have proven to be successful only a few can be mentioned here. One approach consists in treating one or more of the coupled parts of a device or system 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.

Another method is the iterative coupling scheme. Here existing simulators calculate in their specific space and energy domain(s) and communicate with each other along the connecting interfaces according to a "plug-in" algorithm (e.g. Gauss-Seidel relaxation scheme). This method is restricted mostly to small deviations from equilibrium and usually lacks convergence under strong coupling conditions.

These convergence problems can be circumvented by the simultaneous solution of all dynamical equations using special, problem-specific numerical methods (e.g., domain decomposition, non-conforming grids etc.). However, such an 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 "plug-in" approach may be replaced by a Newton iteration, where the required Jacobians are set up only by calls of the single effect simulators. The advantage is that no code modifications on the employed simulators are necessary for the implementation [9].

However, all these approaches will fail in the vicinity of an unstable operating point (as, for example, the well-known snap-down effect in electrostatically actuated microswitches and membrane drives [10,11]). In this situation, homotopy methods are the appropriate means 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 [12,13] along a trajectory of operating points with the homotopy parameter as control variable.

For the sake of brevity, we have to omit the illustration of the above methods by concrete examples. The interested reader will find a multitude of them in the pertinent literature.

4. Coupled-Domain Macromodels of Microsystems

4.1 Lumped Elements and Compact Models

Considering the large numerical effort required for realistic microdevices and systems, the use of continuous field models for the routine analysis becomes easily prohibitive. On the other hand, with a view to assessing the quality of a microdevice in terms of a few characteristic parameters ("figures of merit"), the analysis primarily aims at "concentrated" quantities such as input-output characteristics, response functions and transients, because these quantities characterize the overall performance.

This suggests to reduce the degrees of freedom in the CFM description by proper approximations. In this way it becomes possible to calculate the response function of a real microsystem component by an equivalent but much simpler "compact model" that still reproduces all important physical effects of the device operation with sufficient accuracy, but allows, due to its relative simplicity, the simulation of the device behavior on the system level [14]. To this end, an equivalent lumped element network is derived from the simulated field distributions. The dynamic behavior is now described by a set of ordinary differential equations where the coefficients have been extracted from the physically-based but much more complicated device simulation [15].

The resulting model equations contain parameters, which represent physical, geometrical or technological quantities. They can serve for model calibration and, with the help of additional fit parameters, can be used to reproduce the device characteristics. Sometimes one is led to an explicit analytical expression for the response function, from which easily scaling laws and other useful practical rules can be deduced as guidance for an optimum design. However, for various reasons (complexity of the device geometry, complicated coupling effects) it may turn out impossible to consequently follow this way.

In this case a possible alternative is the numerical simulation of the device behavior by direct use of the original CFM model, employing finite element tools, for instance, and to extract from the discretization mesh an equivalent finite network (cf. sec. 4.3). This approach yields accurate information about the internal operation modes of the device, but the finite network model needs to be set up and interpreted very carefully. Otherwise, important effects may easily be overlooked. The required effort ranges from moderate to prohibitive, depending on the device complexity and the availability of adequate software. Notably the coupling effects require special numerical methods, as already discussed in the previous section.

The choice for the optimum modeling approach depends on technological contraints, the system application of the device, and other factors. If a device is realized in just one version using one given technology, the model may be based on simple curve fitting procedures. But if a device is supposed to have many variants (geometry variations, e.g.), then predictive simulation must be based on a generic "high fidelity" model in order to correctly reproduce the various dependences on technology parameters, operating conditions, geometry etc.

4.2 System Macromodels Represented as Kirchhoffian Networks

Finally, on the system level, all the compact models representing the constituent elements of a microsystem are linked together in order to study the behavior of the system as a whole under the operating conditions of interest. A natural and physically-based methodology for this is provided by a thermodynamic system description [1] in terms of driving forces and resulting fluxes of the relevant physical quantities as expressed in eq. (2). Partitioning the system into blocks and lumping the exchange of flux quantities between adjacent subsystems along common interfaces into single nodes by the use of the balance equations (1) (Fig. 3) eventually yields a full system description as "Generalized Kirchhoffian Network" (Fig. 4), which is governed by generalized mesh rules and node rules for each pair of conjugate fluxes and driving forces and, thus, constitutes a natural approach for system simulation, because the coupling between the different energy and signal domains is governed by basic physical conservation laws for energy, particle numbers, 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.

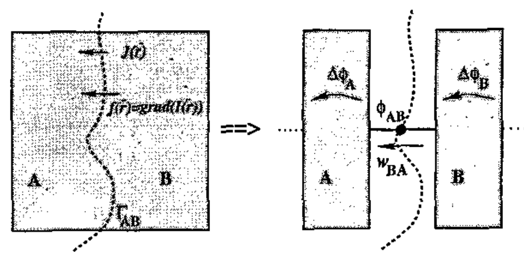

Fig.3: System partitioning into blocks by defining interfaces (left) and lumping the exchange of flux quantities into single nodes (right).

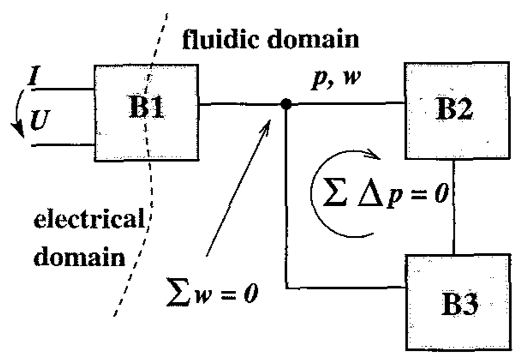

Fig.4: Schematic view of a Kirchhoffian network, coupling different energy domains. The conservation law for the fluidic mass flow w and the hydrostatic pressure p are reflected in sum rules on the nodes and along closed mesh loops.

One should note that only one of two conjugate quantities is determined inside the block, whereas the respective conjugate one can be calculated from the conservation laws governing the network. So the Kirchhoffian network description is, in a certain sense, the natural extension of electric circuit theory, where the branch currents and node voltages are determined by the systematic application of the "current sum rule" at the nodes and the "voltage mesh rule" along a closed loop of the network [16], but now with the extension that also physical quantities other than electrical charge are allowed to flow through the network (cf. Tab. I).

A generic software approach to compact modeling based on Kirchhoffian networks is a hardware description language like VHDL-AMS or Verilog-A [11,17], 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.

energy domain	"across"-quantity	"through"-quantity
electrical	voltage	electric current
thermal	temperature	heat flow
fluidic	pressure	mass flow
mechanical	velocity	force
chemical	chemical potential	particle flow
any	driving force	flux

Table I: Driving forces and resulting fluxes in a Kirchhoffian network.

4.3 Mixed-Level System Macromodels

Not in any case we find a natural decomposition of a coupled-domain continuous-field model in blocks which can be represented by compact models. A typical example is the interaction of a deformable or movable mechanical sub-structure (such as a flexible membrane or a tiltable platform) with a thin viscous fluidic layer, known as squeeze film damping effect [18]. The fluidic continuum model is given by the Navier-Stokes equation which, under the assumption of certain fluid properties and, in particular, a sufficiently large aspect ratio of the lateral structure dimensions to the fluid film thickness, can be replaced by the much simpler Reynolds equation. From the latter, in turn, one could derive an analytical compact model, provided that the mechanical structure has an infinitely extended interface with the fluid film and does not exhibit any holes or perforations. Unfortunately these conditions are almost never very well satisfied, since realistic MEMS structures have complex geometrical shapes, typically with a large number of perforations or slits and a significant influence of the finite structure size on squeeze film damping through edge effects.

Yet, in this situation order reduction can be achieved also for "real life" device structures by a finite network approach. The basic idea is to supplement the overidealizing Reynolds equation, which is still a two-dimensional partial differential equation, by properly chosen boundary conditions at the locations of the perforations, outer edges, and other geometrical non-idealities of the mechanical structure under consideration. These boundary conditions can be represented in terms of fluidic lumped elements (i.e. as compact models), while the Reynolds equation is converted into a Kirchhoffian network, with the compact models attached as correction for the afore-mentioned insufficiences. The netlist of the finite network can be extracted from a FEM model of the device in an automated way (Fig. 5); we end up with a complete Kirchhoffian network of the real device structure, where squeeze film damping is described by a relatively dense mesh with fluidic pressure and mass flow between adjacent nodes as the two conjugate variables, while the device topography is accounted for by the network topology together with the supplementary lumped elements attached.

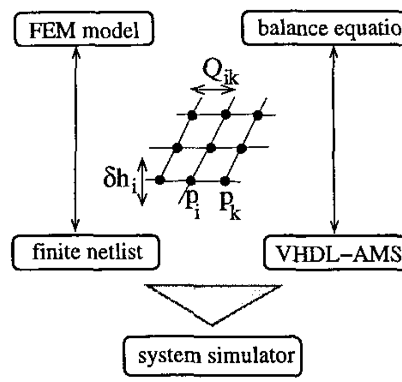

Fig.5: Generation of finite network models formulated in VHDL-AMS for modeling the squeeze film damping effect in microdevices based on the Reynolds equation.

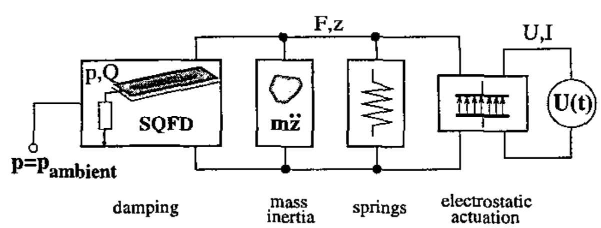

Fig.6: Schematic view of a full system mixed-level model of an electrostatically actuated microdevice affected by squeeze film damping.

The resulting "mixed level" model can be easily combined with finite network or compact models of other parts of the microsystem to form a macromodel that includes all coupled effects and the external electronic circuitry in a uniform description (Fig. 6). In this way, the proposed method offers a high degree of flexibility with respect to the device geometry and the constituent components of the microsystem considered; thus it offers a natural way to manage the coupling to other energy and signal domains by using a uniform simulation environment and commercially available standard system simulators. For more details of this approach, the reader may refer to [18,19].

5. Conclusions and Future Perspectives

Coupled-field device modeling and coupled-domain system simulation have proven to provide very useful or even indispensable support for the development of micromechatronical devices and microsystems, because computer-aided design and performance analysis reduce the number of costly trial-and-error steps and decrease the turn-around times of development cycles. The availability of a easy-to-use predictive "simulation tool box" for microstructures and systems, which provides the functionality necessary for automated parameter identification by closed-loop simulation and thus the capability of easy model calibration, is largely desired, already attempted, and in part realized. We discussed modeling strategies for coupled continuous-field models and multi-energy domain compact models as the essential parts of a comprehensive methodology of bottom-up and top-down microsystem modeling. The practicability and efficiency of such a hierarchical approach has already been demonstrated in the MEMS community by numerous examples.

However, strong efforts must still be made to transform these results in robust, easy-to-use software packages which are ready for use in existing professional TCAD environments. This implies among others that, on the device 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 compact models have to be established, preferably in a simulator-independent generic hardware description language such as VHDL-AMS or Verilog-A. In addition, fast and reliable parameter extraction techniques for compact models, using simulation results from the continuous field level as well as measured data, are required. The corresponding software tools are the indispensable prerequisite for statistical modeling, which in turn addresses such important issues as fabrication yield and reliability.

Acknowledgment

Technical and computational contributions to this work from Dipl.-Phys. Gabi Schrag, Dipl.-Ing. Peter Voigt, Dipl.-Phys. Robert Sattler and Dipl.-Math. Eva-Renate König are gratefully acknowledged.

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