The Art of Modeling Coupled-Field Effects in Microdevices and Microsystems

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ABSTRACT

The rapid progress in microsystems technology is increasingly supported by MEMS-specific modeling methodologies and dedicated simulation tools. These do not only allow the visualization of fabrication processes and operational principles, but they also assist the designer in making decisions with a view to finding optimized microstructures under technological and economical constraints. Currently strong efforts are being made towards a predictive "CAD tool box" for top-down and closed-loop simulation of microsystems. We discuss the most important aspects to be focussed on and practicable methodologies for microdevice and system modeling, in particular the consistent treatment of coupled fields and coupled domains required for setting up physically-based models for full system and mixed-mode simulation, and for the reliable validation and calibration of the models.

MOTIVATION

The recent technical evolution indicates a pronounced trend to products, which are "intelligent" in the sense that they exhibit an integrated self-learning and self-controlling multi-functionality. The practical realization of such system concepts is increasingly based on the potential offered by microsystems technology. Here we recognize a rapid progress in the manufacturing of miniaturized "smart" components with complex functionality, which yet remain amenable to cost-effective fabrication and reliable operation. As a consequence, progressively demanding user specifications can be satisfied, and problem solutions to the real challenges in the development of technical systems become feasible. So the scene is ready to bringing many novel ideas and concepts as new products to the marketplace.

In the development of microsystems we face the problem that intricate trade-off considerations govern their layout and design, and therefore a systematic improvement of the performance is hardly possible without being equipped with a profound expertise in the details of the operation of single microsensor or actuator elements and their interaction as parts of a microsystem 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. While the traditional experimental way of developing new microdevices involves several design and fabrication cycles, until the given specifications are satisfied, computer-aided design (CAD) can reduce the number of costly trial-and-error steps and decrease the turn-around times of development cycles. Hence, modeling and numerical simulation is widely accepted as cost-effective and time-saving alternative approach.

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. 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.

Actually there are two main objectives for modeling and numerical simulation [1]: Enhanced physical understanding of operational principles ("verification of concepts", "visualization of physical effects") and aid in making decisions during (re-)design ("analysis of design variants", "study of trade-offs"). The long-term objective is the fully computer-based development of microdevices or complete microsystems according to user-supplied specifications.

The evident prerequisite for the technical realization of this idea is the availability of a set of efficient simulation tools, which fit in with today's far advanced design environments used in the semi-conductor industry and, in particular, are conform with the widely accepted bottom-up and top-down modeling hierarchies. In this way, just as computer technology radically changed the economics of integrated circuit design over the last decade, computer-aided design is likely to change the economics of microsystems design and manufacture.

SPECIFIC ASPECTS OF MEMSMODELING

In spite of what they have in common, there are several aspects in which microsystems technology differs largely from integrated circuit (IC) technology. Integrated circuits are composed of a quite limited number of elementary device structures, fabricated by means of well-established and quasi-standardized design rules and process technologies. In the field of MEMS technology, however, an ever-growing variety of different device types have emerged, based on rather unconventional design methods and a large number of widely differing (and sometimes brand new) 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 devices which, however, exhibit a high functional complexity based on quite sophisticated and involved physical operating principles.

The complexity of microsystems originates in particular from the afore-mentioned complicated coupling between different energy and signal domains which, on the one hand, is the inherent and much desired property of any sensor or 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. Therefore the computational effort as well as the time spent into model development, validation, calibration, and parameter extraction have to be carefully adjusted to the actual needs, as it has been proposed by the concept of "tailored modeling" [2].

As the state of the art in modeling, simulation, and design optimization is far advanced in the world of microelectronics, it makes sense to adopt the well-tried methodologies for model generation and parameter extraction used in IC technology. Of course, the particular demands on the models arising from their dedicated application to MEMS must be properly accounted for. Implementation in a "CAD toolbox for MEMS", similar to the well established TCAD frame-works 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 [3-6] and appear quite promising, even though their application is still restricted with respect to the geometric and functional complexity of a microdevice and the included coupling effects.

COUPLED-FIELD MODELS OF MICRODEVICES

The most rigorous approach to develop a MEMS model is the detailed physical analysis of its operation principles. To this end, the physical operation of single microdevices as well as their interplay as constituent elements in a microsystem are described on the level of continuous-field models (CFM) which couple the relevant field quantities (mechanical, thermal, electric, magnetic, optical, chemical...) consistently in terms of a (typically quite complicated) system of partial differential equations. On this level, after selecting the proper physical models 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. 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 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 [7].

These convergence problems can be circumvented by the simultaneous solution of all dynamical equations using special, problem-specific numerical methods (e.g., domain decomposition, nonconforming 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 [8].

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 membrane drives [9]). 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 [10, 11] along a trajectory of operating points with the homotopy parameter as control variable.

For the sake of brevity, we will omit the illustration of the above methods by concrete examples. The interested reader will find a multitude of them in the pertinent literature; for instance, a sophisticated coupled-field analysis of distributed electro-mechanical parasitics in industrial CMOS pressure sensors has very recently been presented in [12]. Instead we will concentrate on the system aspects in the following.

COUPLED-DOMAIN MODELS FOR MICROSYSTEM SIMULATION

Compact Models

Since on the device level simulation is based on a continuous-field model, which is mathematically represented by a coupled system of partial differential equations, the final result is the spatial distribution of the respective field(s), possibly as a function of time. However, 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 integral quantities such as input-output characteristics, response functions and transients, because these quantities characterize the overall performance.

To this end, the degrees of freedom in the CFM description have to be reduced by proper approximations. This makes it 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 correctly, but allows, due to its relative simplicity, the simulation of the device behavior on the system level [2]. In this way 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.

The resulting model equations contain parameters, which represent physical, geometrical or technological quantities. They can serve as basis functions 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 [13]. However, for various reasons (complexity of the device geometry, complicated coupling effects) it may turn out impossible to consequently follow this way.

A possible alternative then is the numerical simulation of the device behavior by direct use of the original CFM model, employing finite element tools, for instance. This approach yields accurate information about the operation principles of the device, but the finite element model needs to be set up and interpreted 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 easiest way to generate compact models is pure curve fitting, based on measured data or on CFM simulation results. Such a model, if not supported by a physical description of the device operation, lacks all predictive capabilities and can hardly be used to inter- or extrapolate in the space of design parameters and operating conditions.

The choice for the optimum modeling approach depends on technological constraints, 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 curve fitting procedures. But if a device would have many variants (geometry variations, for instance), then a generic model is required that correctly reproduces the dependencies from technology parameters, operating conditions, geometry etc.

Kirchhoffian Network Description

Finally, on the system level, all the compact models representing the constituent elements of a micro-system 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 thermo-dynamic system description in terms of driving forces and resulting fluxes of the relevant physical quantities [2]. Partitioning the system into blocks and lumping the exchange of flux quantities between adjacent sub-systems along common interfaces into single nodes (Fig. 3) eventually yields a full system description as "Generalized Kirchhoffian Network", 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.

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 [14], but now with the extension that also physical quantities other than electrical charge are allowed to flow through the network (cf. Tab. I).

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

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

The Kirchhoffian network description is also useful for testing the function of one (or a few) system element(s) on the device level (i.e. continuous-field level), when they are embedded in the full system environment (for instance, a sensor element coupled to the electric circuitry). To this end, a few selected single components are modeled using the device-level (CFM) description, while the rest of the system is treated using conventional system-simulation techniques. This approach is referred to as "mixed mode" simulation, since physically-based numerical models and semi-analytical compact models are used simultaneously.

A generic software approach to compact modeling based on Kirchhoffian networks is a hardware description language like VHDL-AMS [15], which constitutes a standardized model interface in analog network simulators and, furthermore, allows the description of arbitrary physical energy and signal domains in addition

MODEL VALIDATION AND CALIBRATION

In order to establish a quantitative correspondence between simulated device and system operation on the one hand and the real behavior on the other hand, the simulation models have to verified and calibrated. Each of the above-discussed modeling approaches requires an appropriate extraction technique and, in return, the limitations of different extraction methods may influence the decision for a specific modeling strategy.

In case of a modeling methodology based on data fitting, model verification on the system level is simply a test if the simulated data reproduces the input data from measurement or CFM simulation within the required accuracy. The appropriate extraction technique would be a global error-minimizing algorithm. The advantage is a very fast setup of the extraction, but one pays with rather lengthy optimization runs. The extracted parameters can hardly be used for predictive simulation or statistical analysis, and a physical interpretation is quite often impossible.

In the case of physically based models, a global minimization scheme could easily erode the physical content of the model parameters. Instead an extraction scheme utilizing direct extraction steps and carefully tuned local minimization needs to be employed. Comparing in detail the results of simulated and measured operating behavior of special test structures or prototypes allows one to decide whether the simulation can be accepted or not. Of course, after the first run through the simulation sequence from the device level up to the system level, the verification procedure is likely to fail in consequence of improperly chosen models or model parameters or due to in-accurate values of the material coefficients. Identifying these deficiencies and correcting for them by application of a suitable error-minimizing algorithm as proposed by the concept of "inverse modeling" [16], the discrepancies in the verification step will progressively become smaller until, after sufficient iterative improvements, acceptable agreement between the real and the simulated device and system operation is achieved.

This procedure, called "closed-loop simulation"(cf. Fig. 1), is the decisive step in making a simulation tool box capable of computer-aided design of micro-devices and systems in the genuine sense. If convergence is attained on all model levels, the physical models incorporated in the simulation system can be regarded as validated for the technological processes and structures under consideration. Otherwise, some of the underlying model assumptions are presumably inadequate and must be revised.

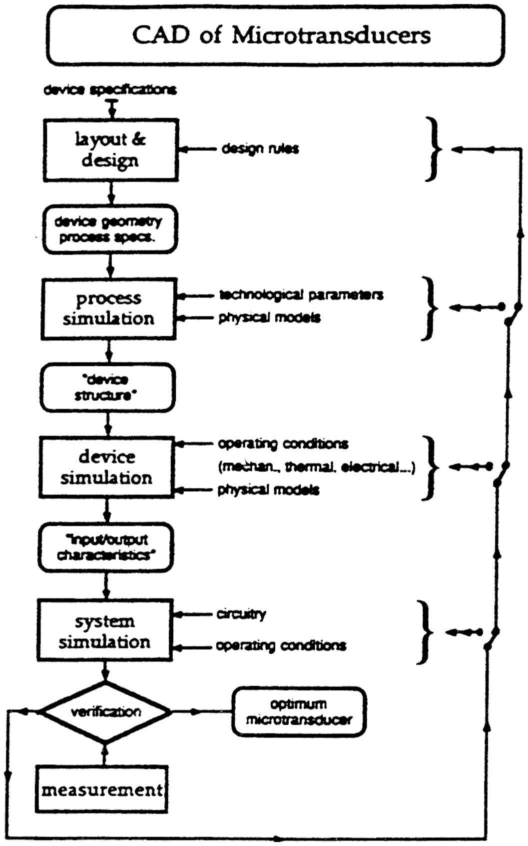

Fig. 1: Functional sequence of model levels in the closed-loop simulation of microsystems (adopted from [1])

It is a peculiarity of microstructures that the physical properties may be dependent on the fabrication process. In this case, measured values are possibly available from the microstructure manufacturer but, of course, applicable only under the specific constraints which underlie the respective manufacturing process. Consequently, whenever the process conditions are changed, all involved physical models have to be revalidated, preferably by means of predefined test structures. For easy management and access to these voluminous data sets, process-oriented material property databases are currently built up (as, for instance, in the German High Priority Consortium SIMIKO [17]).

Provided the simulation system has successfully passed the validation procedure, the really existing test structure used for the calibration of the model parameters may now be replaced by a virtual device imagined by the designer, using the specifications as desired by the customer. Again closed-loop simulation is iterated until the desired operating behavior is reproduced by the simulation system, thus providing a recipe for the manufacturer how to design the real device and how to operate it in the real environment. In this way, the vision of automated microsystem design might become real in future.

CONCLUSIONS

Coupled-field device modeling and coupled-domain system simulation have proven to be definitely useful or even indispensable for the development of inexpensive MEMS components and micro-systems with competitive performance, because computer-aided design can reduce the number of costly trial-and-error steps and decrease the turn-around times of development cycles. The availability of an easy-to-use predictive "CAD 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.

Now efforts must be made to transform these results in robust, easy-to-use software packages, which are ready for use in existing professional CAD environments. This implies 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. In addition, fast and reliable parameter extraction techniques for compact models, using CFM simulation results 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.

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