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Coupled Problems in Microsystem Technology

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COUPLED PROBLEMS IN MICROSYSTEM TECHNOLOGY

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SUMMARY

In microsystem technology, the numerical simulation of coupled problems is one of the principal challenges. We present a classification of the most important occurring couplings, and we give a survey of existing solution techniques with emphasis on the so-called *partitioned solution*. Here, there is no joint model, neither continuous nor discrete, but the coupled problem is solved by an outer iteration for the coupling and by arbitrary inner solution processes for each single problem. The coupling is done via changed boundary conditions, geometries, or parameters after each step of iteration. This approach seems to be advantageous, since its modularity allows the use of existing and efficient codes for each sub-problem. Thus, only the outer iteration has to be organized with some kind of interface for the coupling. Furthermore, this technique is perfectly suited for parallelization, especially for the use of (heterogeneous) workstation clusters. For the simulation of a micro-miniaturized two-valve membrane pump, first numerical results are presented.

INTRODUCTION

In the last years, the advances in semiconductor technology concerning both the numerical simulation and the production of microchips have led to growing endeavours to profit from the experiences and progresses there in other fields of industrial relevance, too. Especially the efforts for micro-miniaturized sensors like acceleration sensors in modern airbag systems and for microactuators like microvalves or micropumps in medicine, e. g., finally resulted in what we call microsystem technology today. Since a realistic prototyping and the following production are often very costly, the numerical simulation of such microsystems turns out to be imperative.

When we try to tackle the numerical simulation of a microsystem, we learn immediately that we can't avoid to deal with the numerical treatment of coupled problems. There are three main reasons for the fact that, here, the coupling of different physical effects (structural dynamics, fluid dynamics, heat transfer, or electromagnetics, e.g.) and the coupling of the physical level with the system level (integration of a device simulation into the simulation of the surrounding electric circuit, e. g.) are more frequently encountered than in the macro world: First, aspects of scaling often lead to a dominance of surface effects over volume dependent effects. Second, especially in sensors a lot of different physical phenomena are used for signal conversion. Finally, in some microsystems different physical effects may have an influence on each other, which can result in so-called cross talk effects between different closely related conductors, e. g.

Furthermore, the variety of physical effects possibly involved in a microsystem and the resulting great variety of possible couplings show the disadvantages of the standard approach of defining a model for one particular coupled problem or one class of coupled problems and of finding a way for its numerical treatment by adding new features to existing programs. The development of such complex models usually takes a lot of time, and the resulting codes can often be neither applied easily to other problems nor extended in a simple manner if growing accuracy requirements demand a more precise model, e. g. This is the reason why modular solution techniques based on the connection of different existing codes for different sub-problems seem to be a very promising approach for an efficient numerical simulation of coupled problems.

MICROSYSTEMS

As mentioned above, a microsystem could be defined as the integration of microelectronic components like integrated circuits and non-microelectronic components like micromechanical sensors or actuators into one complete system. Typically, the overall dimensions of such systems are in the range of a few thousand μm. The principal structure of a microsystem is illustrated in the following figure (1).

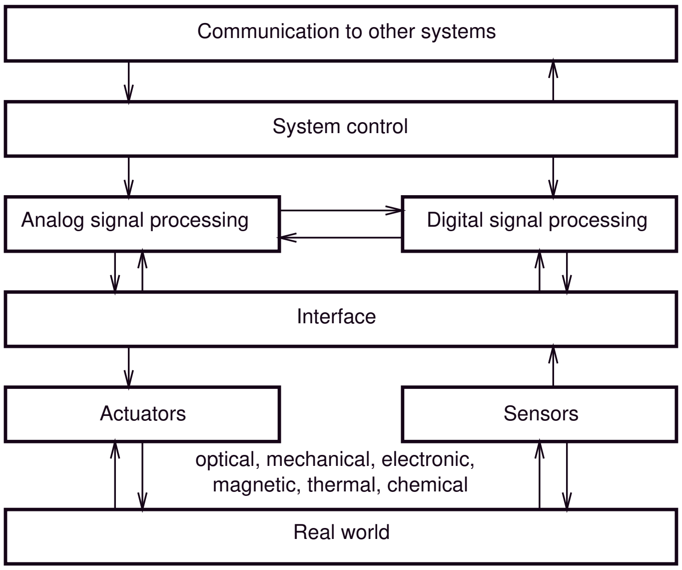

Fig. 1 Principal structure of a microsystem.

An example for a microsystem which is in the development stage now is the future generation of airbag systems. These systems must combine sensors for measuring the acceleration and electric circuits for processing the measured data and comparing them with the reference data in order to decide whether the airbag has to be blown up or not. Finally, if a crash is indicated, the actuators must inflame the explosive. In such complex systems, some components like the so-called force balance accelerometers [13] can be microsystems themselves (sensors, actuators, or electronic control units). Since a microsystem contains components from different disciplines like microelectronics or micromechanics, the term *microelectromechanical system* to describe such devices is often used.

Starting out from the above interpretation of a microsystem, we can think of microsystem technology as a combination of different microtechnologies by the application of system technologies like packaging, interconnections, and testing. Moreover, especially in the context of chemo- and bio-sensitive materials or piezo technologies, material sciences are in the centre of interest, too. Finally, one of the main tasks of system technologies is the development of methods and tools for the computer based design of the whole microsystem (cf. MEMCAD [22]).

The numerical simulation of the behaviour of single components and of the whole system is very important during the design process, because a development based on experiments only would require the fabrication of (very expensive) prototypes and the measuring of the critical parameters. Since the sensors used for that are usually bigger than the whole system to be measured itself, this is often not feasible. Generally, the numerical simulation of the component behaviour means the solution of the partial differential equations which model the most relevant physical effects of this special device, e. g. the mechanical deformation of a cantilever. This kind of simulation is called simulation on the physical level. To describe the behaviour of the whole system, it is necessary to make a more abstract model which can, usually, mathematically be described by systems of ordinary differential equations. An example for this is the simulation of electric circuits. In the future, couplings between different levels like the physical and the system level will have to be taken into account to an increasing degree, especially because of growing requirements concerning accuracy and reliability.

COUPLED PROBLEMS

In the macro world, coupled problems and their numerical treatment have a rather long tradition that goes back to the late sixties. The main emphasis has always been put on topics like fluid-structure interaction, thermo-elasticity, or soil-pore interaction. For fluid-structure interaction, e. g., the examples range from aero-elasticity in the design of aircraft wings to reactor safety [33] and from the earthquake-proof construction of dams [19] to examinations concerning the vibration of bridges — a problem that attained a lot of popularity after the spectacular collapse of the Tacoma bridge in 1940.

This variety of examples for coupled problems from all kinds of areas of application led to a very broad interpretation of the term *coupled problems* and to the development of very different techniques for their numerical treatment [11, 16]. A first kind of a unifying approach was done by Zienkiewicz [32]. There, a coupled problem is defined as a set of n bidirectionally combined sub-problems $\mathcal{P}_i$, $1 \leq i \leq n$,

$$[L_i(x_1, ..., x_{i-1}, x_{i+1}, ..., x_n)]\,(x_i) = f_i(x_i; x_1, ..., x_{i-1}, x_{i+1}, ..., x_n), \tag{1}$$

with operators L_i, right hand sides f_i, unknowns x_i, and parameters $x_1, ..., x_{i-1}, x_{i+1}, ..., x_n$. Here, the principal requirement is the bidirectional coupling, i. e. the fact that there is neither any possibility for an explicit elimination of parameters which link the different sub-problems nor any way of an independent solution of any $\mathcal{P}_i$.

Following this definition of a coupled problem, Zienkiewicz in [32] also presents a first classification of coupled problems. He distinguishes between two classes of problems: those with totally or partially overlapping domains and those with different domains. In the first case, the coupling takes place via the differential equations that, usually, refer to different underlying physical phenomena. The second class, however, is characterized by a coupling that occurs on the domain interfaces, i. e. via the boundary conditions.

Here, a further distinction is made between problems with different underlying physics or different variables (fluid-structure interaction or structure-electrostatics interaction, e. g.) and problems with identical physics and variables (structure-structure interaction, e. g.).

In contrast to the above definition of a coupled problem by Zienkiewicz, the terms *coupled problems* or *coupled methods* are often used in a broader sense. Then, these also include the so-called mixed problems, which allow both a reducible coupled and an irreducible single problem formulation, but also domain decomposition methods, where all $\mathcal{P}_i$ describe identical physical phenomena on different sub-domains, or the coupling of different discretization schemes like finite element and boundary element methods. Furthermore, even systems of linear or non-linear algebraic equations or ordinary differential equations, to some extent, can be seen as coupled problems.

Finally, it must not be forgotten that the topic of coupled problems has been tackled by researchers from other disciplines than numerical simulation. For instance, the field of multidisciplinary design optimization that is concerned with how to analyse efficiently and design optimally a system governed by multiple coupled disciplines or made up of coupled components works on coupled problems, too [1]. Since the approaches discussed there come from the theory of systems, they are much more generally orientated and do not start from a specific problem.

When we are looking for efficient modular strategies to deal with the numerical solution of coupled problems in a flexible manner that is independent of a specific problem, those various approaches from other disciplines, but also methods known from the iterative solution of large systems of linear equations [10], e. g., can be very helpful. Furthermore, since we want to solve coupled problems from microsystem technology, we have to take into account the special conditions and requirements of the micro world.

COUPLED PROBLEMS IN MICROSYSTEM TECHNOLOGY

The importance of cross coupled effects in micro technology results from three different facts which are closely related to what characterizes a microsystem.

Most of the couplings observed on the physical level can be seen as a consequence of the scaling behaviour of the basic quantities length, surface, and volume. When the dimensions of a system represented by the characteristic length L tend towards zero, the surface and the volume tend towards zero like L^2 and L^3, respectively. Because of that, for decreasing L, there is a growing importance of all terms proportional to the surface. Consequently, surface forces like pressure or electrostatic loads dominate volume forces, for example magnetic or mass dependent loads like inertial forces. Coupled problems resulting from these scaling properties naturally belong to the second class in the scheme of Zienkiewicz, because the interaction occurs only on the domain interfaces.

Especially in sensor design, a lot of different physical phenomena have often to be used for the conversion of the quantity to be measured into a signal which is well suited for further data processing steps. This characteristic transformation of an input signal into an (electric) output signal can be used for a definition of sensors [8]. Here, a unidirectional coupling of different effects is the basic principle of a sensor. Since some of the phenomena used for signal conversion are closely connected, a bidirectional coupling can not always be avoided.

The third reason for the importance of couplings in the micro world stems from the high integration density caused by the small overall dimensions. For example, in so-called smart sensors where the sensor device is combined with electric circuits for the signal conversion and for the compensation of secondary effects, the heat emission of the electronic device can cause thermal strains in the mechanical part of the sensor, if the distances are too small. Furthermore, the field of the so-called electromagnetic compatibilities (EMC) deals with mutual influences or cross talks between electric conductors. Especially problems of this type could require the combination of the simulation on the system level (circuit behaviour) and the simulation on the physical level.

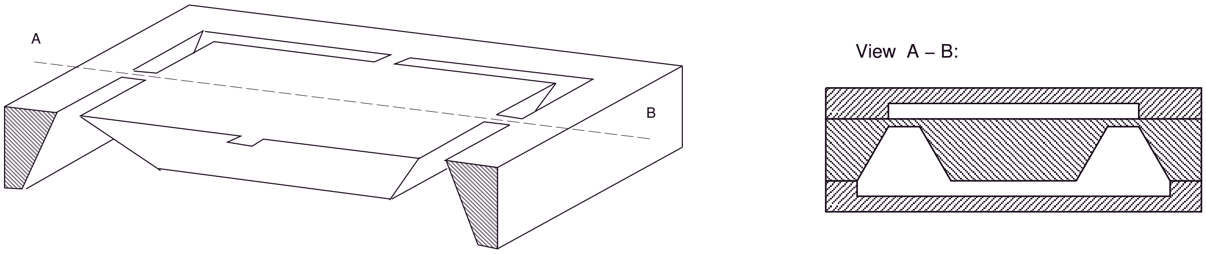

Fig. 2 Piezoresistive accelerometer with seismic mass.

Now, let us look at some micromechanical components whose behaviour is dominated by couplings between different phenomena on the physical level. Figure (2) shows the basic structure of most of today's accelerometers. Here, the deflection of a movable mass caused by the acceleration forces and determined by different possible techniques (capacitive principle, piezoresistive films) is used as a measure for the actual acceleration. In fact, each sensor of this type is a resonator with its main degree of freedom in the direction in which the acceleration shall be measured. The damping behaviour of such a device is strongly influenced by the pressure and the viscosity of the surrounding gas. In [27], the influences of the different parameters such as the distance of the movable mass from the ground plate or the viscosity of the surrounding fluid are analysed, and it is shown that there is a close connection between the fluid flow and the structural dynamic problem. Furthermore, a mathematical model to handle this problem like a squeeze film damper is suggested. The basic idea of this approach, the modeling of the fluid flow with the Reynolds equation from lubrication theory [24], goes back to the sixties [9]. Note that, for lubrication problems, a lot of interesting (and modular) solution approaches have been developed [11, 12, 15].

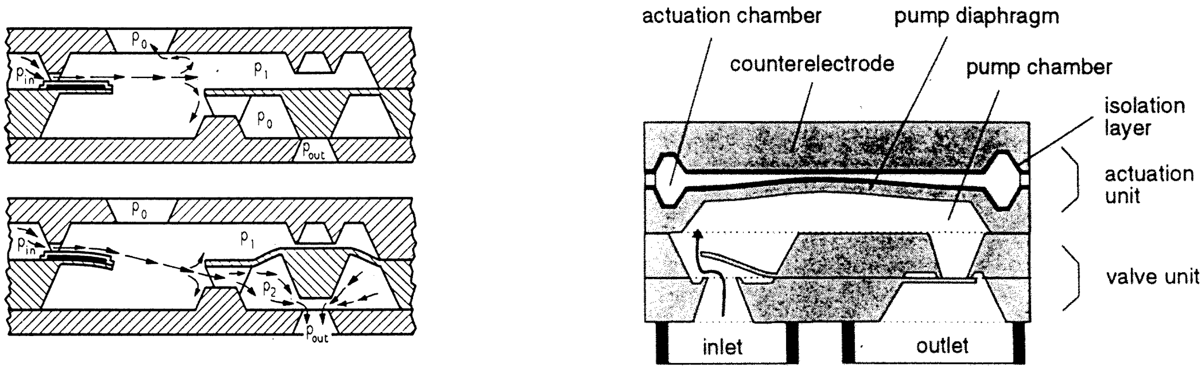

Fig. 3 Hydraulically actuated valve (left, taken from [26]) and two-valve membrane micropump (right, taken from [31]). The micropump has outer dimensions of $14.5 \times 8.5 \times 1.43\,\mathrm{mm}^3$. It is designed for flow rates of about 75 ml/min and a system pressure level of about 6 bar.

Other examples for problems with fluid-structure interaction in micro technology are shown in figure (3). Here, the fluid flow has to be modeled by the complete Navier-Stokes equations. Micropumps like the one of figure (3) will have a broad range of applications in the future (medical drug infiltration systems [23], microfluidic systems for chemical analysis, or environmental applications, e. g.).

To get an overview of the cross coupling problems in microsystem technology, a systematic analysis including both an application based and a theoretical approach with the derivation of the mathematical models of the different considered single field effects in a unique notation has been done. As a result, the 'coupling matrix' in figure (4) summarizes the different couplings on the physical level. In the lower diagonal part, the results from the theoretical approach are indicated, and the upper part shows examples from the different areas of application. As already mentioned above, some types of microsystems require to consider the interaction of phenomena occurring on the physical level with those on the system level. Simulation problems with both kinds of phenomena have turned out to be typical for microsystems (see figure (5)).

components / kind of coupling	**s**tructural dynamics	**h**eat conduction	**f**luid dynamics	**e**lectromagnetics
structural dynamics		- resonators (thermally induced high frequency vibrations) - thermal actuators	- accelerometers - gyroscopes - valves, pumpes	- sensors with capacitive detection - electrostatic and piezoelectric actuators
heat conduction	thermo-elasticity h→s: material law s→h: energy dissipation		- microcooler - flow- and thermal sensors	- thermopiles (electrical heating with integrated resistors) - thermal actuators (pump actuation, resonators)
fluid dynamics	f→s: surface forces s→f: - geometry - boundary cond.	coupled by the energy equation		- sensors and pumps working with the electrohydrodynamic principle
electromagnetics	e→s: surface and volume forces s→e: - geometry - moving conductor	e→h: electromagnetic loss h→e: material properties	electrohydrodynamics e→s: surface and volume forces s→e: - geometry - moving conductor	

Fig. 4 Coupling matrix on the physical level.

A SOLUTION APPROACH

The broad spectrum of applications of coupled problems and the heterogeneous way they appear in different disciplines led to numerous suggestions for their numerical treatment [21]. Among these approaches that have nearly all originally been developed with one special problem in mind and have afterwards been generalized, it is possible to distinguish two classes (see figure (6)).

First, the connection of the different mathematical models via their coupling condition

components / kind of coupling	circuit simulation	multibody dynamics	structural dynamics	heat conduction	fluid dynamics	electro-magnetics
circuit simulation		mechatronic systems - airbag - control units of combustion engines	- smart sensors - force balance accelerometer	thermal design of electronic circuits with respect to placement		electromagnetic compatibility (EMC) on circuit level
multibody dynamics	c→m: control theory m→c: system response		elasticity of components in multibody systems, e.g. robot arms		simplified model of the acceleration sensor	multibody motion in an electrostatic field, e.g. motors, generators
structural dynamics	coupling via additional effects, e.g. electrostatics	boundary conditions				
heat conduction	h→c: temperature dependent components c→h: heat source			Cross coupling on the physical level		
fluid dynamics		similar to fluid-structure interaction				
electro-magnetics	current flow ↕ field around conductor	e→m: surface and volume forces m→e: moving conductor				

Fig. 5 Coupling matrix on the system level.

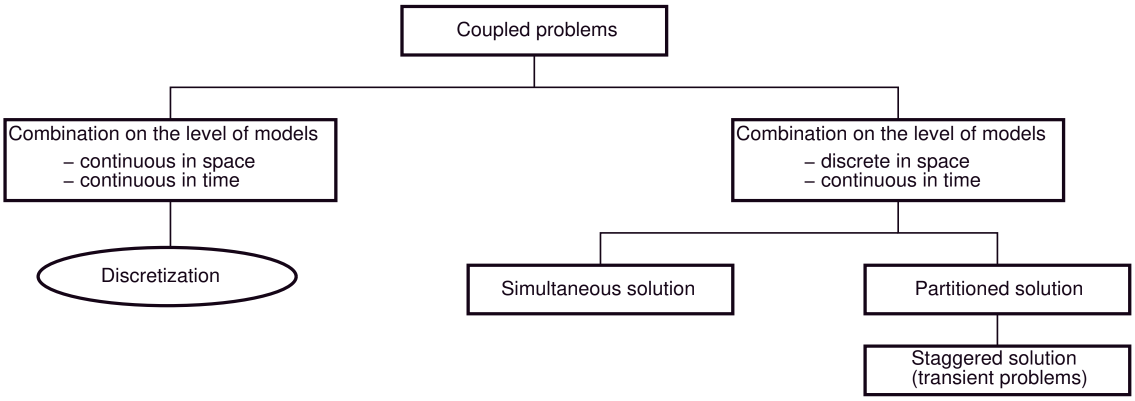

Fig. 6 Classification of the solution approaches.

is the most natural way and results in a system of partial differential equations with appropriate boundary and initial conditions. An example for that is thermo-elasticity [2]. Here, the equations from structural dynamics which regard thermally induced strains and temperature dependent material properties have to be coupled with the heat equation, in which the source term is given by a time dependent change of the strain tensor. An alternative way of deriving combined mathematical models is that of considering the energy functional [6], which finally leads to bond graph techniques [20, 25]. Used especially for the simulation of problems in thermo-electricity, the so-called *tailored modeling* [28] starts from a mathematical model that contains each relevant effect of the considered class of problems. Thus, the couplings are taken into account automatically. In order to reduce the model, only the important variables are considered in the further modeling steps, i. e., the model is tailored according to the given problem.

In contrast to the realization of the coupling on the continuous level, we can also couple the different semi-discrete models (cf. figure (6)) which have the form of algebraic equations if the problems do not depend on time, and which are ordinary differential equations otherwise. The resulting block-structured systems can be handled in two different ways.

In the first method called *simultaneous solution*, standard methods like Gauss elimination or block Gauss elimination in the case of linear equations are used to solve the equations of the combined model. A general disadvantage of the simultaneous solution is the fact that symmetry and sparsity of the resulting matrix may get lost due to the coupling terms even if each single problem is symmetric and sparse. Furthermore, in the case of time dependent problems, the system of ordinary differential equations which results from the combination of two problems which show different time behaviour could be stiff.

To avoid these difficulties and to get a modular approach, the so-called *partitioned solution* shown in figure (7) has been developed [4, 5]. Here, there is no joint model, neither continuous nor discrete, but the coupled problem is solved by an outer iteration for the coupling and by arbitrary inner solution processes for each single problem. The coupling is done via changed boundary conditions, geometries, or parameters after each step of iteration. Concerning the organization of the outer iteration, Jacobi-, Gauss-Seidel-, or SOR-type methods are the state of the art. In the latter case, the relaxation parameters are normally fixed by experiment and strongly problem dependent. The convergence behaviour of such methods can not be guaranteed in general [29] and has been studied for a few specific problems only.

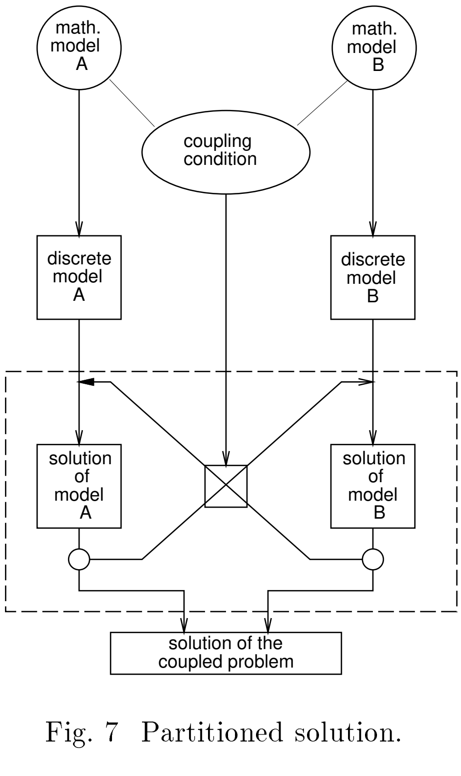

Fig. 7 Partitioned solution.

Whereas most of the techniques introduced so far have been developed starting from a specific problem, the partitioned solution leads to a more general and methodical point of view. Following this idea, we suggest an approach in which the coupled solution shows the same structure as the coupled problem to be solved. We start from a description of the coupled problem by its different underlying single field phenomena $\mathcal{P}_i$, represented by the operators L_i of their mathematical models (cf. (1)), and the corresponding coupling operators C_{ij} for the couplings from $\mathcal{P}_i$ to $\mathcal{P}_j$. For the numerical treatment of the whole coupled problem, each $\mathcal{P}_i$ gets its own solver S_i attached, and C_{ij} and C_{ji} are taken into account by an appropriate iterative strategy It_{ij} (see figure (8)).

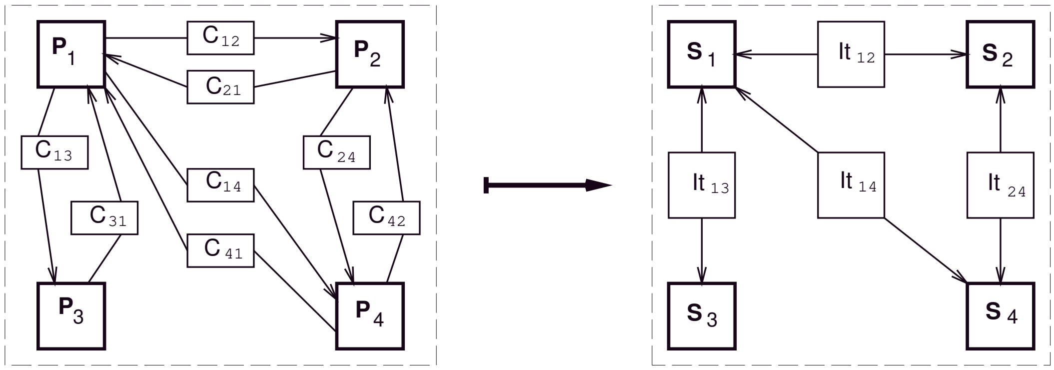

Fig. 8 Coupled problem (left) and its coupled solution (right).

The realization of such an algorithm can be seen as a typical task of scientific computing, because aspects from numerical analysis, computer science, and the respective area of application (microsystem design, e. g.) have to be considered.

From the point of view of numerical analysis, the construction of outer iteration schemes for both stationary and time dependent problems as well as the development of strategies for the variable transformation at the problem interfaces (non-matching discretizations with self-adaptive sub-problem solvers, e. g.) are in the centre of interest. Furthermore, we need error indicators and estimators for the overall procedure in order to be able to decide which sub-problem has to be solved more exactly.

Considering the aspects of computer science, one has to organize the communication between the different solvers at the interfaces as well as the control of the overall procedure. Moreover, there is the question of how to implement the coupled solution process in a heterogeneous computer environment when sub-problem solvers with licences restricted to special nodes have to be used.

Finally, the main task on the part of the applications is the preparation of appropriate mathematical models for the single effects and for the couplings between them. Especially for the derivation of the coupling operators C_{ij}, there are often several alternatives, and the choice of the most suitable one may depend on the respective outer iteration strategy.

The main objective of our work in that context is to analyse the connections between the different components like outer iteration scheme, single field solvers, coupling and interface operators, and so on, in order to optimize the overall procedure introduced in figure (8). As a result of such an analysis, we want to get some kind of list of requirements which should be fulfilled by each single field solver to facilitate its efficient use in coupled solution processes. On the other hand, if a problem and the corresponding available single field solvers are given, we want to provide criteria for the proper decision which solution strategy should be used.

In micropumps like the one shown in figure (3), different kinds of couplings can be observed. The development of one single model for the whole device would require the consideration of the electrostatics-structure interaction used in the actuation unit and the fluid-structure interaction in the valve unit. Furthermore, the actuation unit is coupled to an electric circuit in order to control the flow rate. For a first model, however, we restrict ourselves to the fluid-structure interaction and model the actuation unit via velocity boundary conditions. Furthermore, since our main interest are the algorithmic aspects of coupled solution, we only look at the 2D case, first. The following figure (9) shows the physical model used and explains the principal structure of such a device.

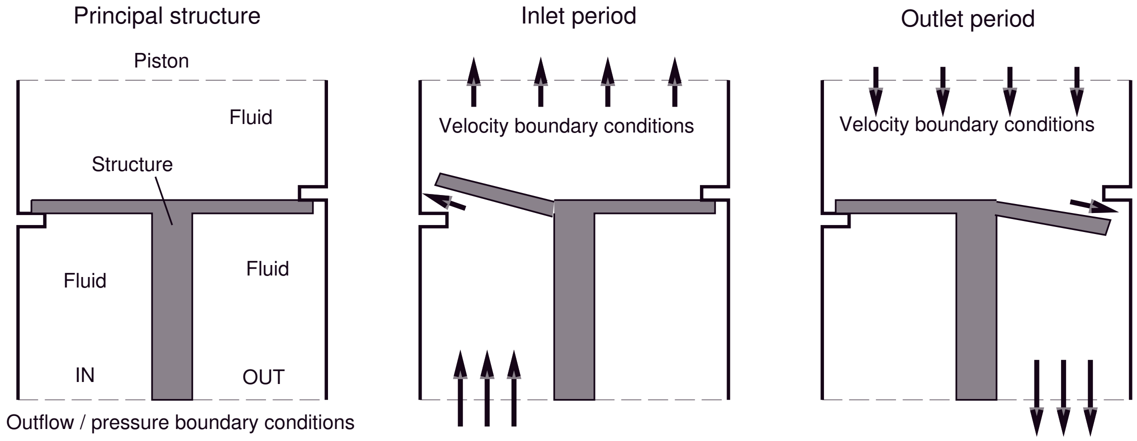

Fig. 9 Principal structure and functional description of the model.

First, we concentrate on the stationary form of the problem: The fluid flow influences the structure via pressure loads at the wetted surface of the structure (interface). As a result, the corresponding coupling operator is given as the identity restricted to the interface nodes. On the other hand, the deformation of the structure changes the geometry of the fluid domain. This leads to a non-linear form of the coupled problem even in the case of a linear model for the fluid flow like a potential flow, because changes in domain geometry result in a changed discretized form of the fluid flow operator.

For modeling the fluid problem, the incompressible form of the stationary Navier-Stokes equations is taken. Based on measured flow rates and the underlying geometry of the flaps [30], the Reynolds number was estimated to take values of about 300. Laminar flow conditions are supposed for the whole domain and for each position of the valve. Note that this might be unrealistic, especially around the valves, but on the other hand, the small dimensions and an appropriate choice of the geometry like in figure (3) should help to prevent turbulence. Anyway, it is a crucial task to find an accurate physical model for the flow around an opening flap, because the flow conditions change form squeeze film flow for very small slots (Reynolds equation from lubrication theory) to the one which can be described by the full Navier-Stokes equations only.

For the flow simulation, a Navier-Stokes solver based on the MAC-technique and implemented by Griebel et. al. [3] was used. The main advantage of this code from our point of view is that it makes possible a very simple and flexible handling of complicated geometries and moving boundaries. For a detailed description of the code and its main properties, see [3].

To calculate the deflection of an arbitrary elastic structure in 3D caused by a pressure distribution on the surface, the equations of linear elasticity (Navier equation) have to be used. Due to the special geometry (high aspect ratio of the flap length to its thickness), the use of the simpler plate equation is possible. For 2D problems, this results in an ordinary differential equation known from the bending of beams. Thus, for the description of the mechanical part of the valve behaviour, the model is based on the one of a cantilever fixed at one end and loaded by a continuous pressure distribution on its surface.

To get an idea of the strength of the coupling and the general flow situation inside such a device, the modeling was done in three main steps. First, the flaps were taken as non-flexible plates opened and closed in order to control the flow inside the pump (see figure (9)). In the second step, the deformation of the valves was calculated using the plate equation, which can be solved analytically (see figure (10)).

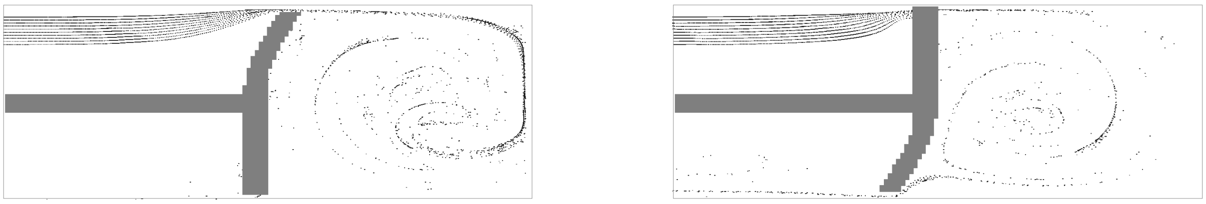

Fig. 10 Streaklines during inlet (left) and outlet (right) period.

Finally, we modeled the deformation of the flaps assuming a plain strain problem. For this simulation task from structural mechanics, we used the commercial finite element package ADINA. Now, the coupled solution was realized with a partitioned solution scheme like the one of figure (7). For the first tests, each iteration step started with the creation of a new input file based on the results of the previous run. Note that this is not necessary, because in the structural problem only the right hand side (load vector) has to be modified, whereas the factorized stiffness matrix can still be used. First of all, Jacobi- and Gauss-Seidel-type iterations were tested. As in [29], a strongly problem dependent convergence behaviour could be observed. For the coupled stationary simulation of the inlet valve, table (1) shows the influence of the stiffness of the valve itself (Young's modulus) and the influence of the viscosity of the surrounding fluid (Reynolds number) on the number of (outer) iteration steps that are necessary till the flap has reached its final (open) position or a state where it alternates between two or three neighbouring positions.

CONCLUDING REMARKS

In this paper, we gave a short survey of both the relevance and the numerical treatment of coupled problems in microsystem technology, and we presented a modular strategy based on the partitioned solution approach as well as first numerical results concerning the simulation of a two-valve membrane pump. We can summarize that the coupled problems which have been observed in the micro world up to now are very heterogeneous. It depends strongly on the specific problem whether the coupling has to be considered or not and which mathematical model has to be used for an efficient numerical treatment. Another interesting problem which shall not be discussed in detail here is the question of the validity of the classical models from the macro world. Especially for flow problems with low Knudsen numbers, e. g., a modification of the models is necessary [17].

Table 1 Dependence of the convergence behaviour on problem parameters.

Outer iteration	**Problem parameters**		**Number of iterations**
	Young's modulus	Reynolds number	*: alternating states
Gauss-Seidel	$2.0 \cdot 10^{11}$	100	7
		200	10
		333	8^*
	$1.5 \cdot 10^{11}$	100	9^*
		200	13^*

Of course, one of the most essential parts in partitioned solution is the outer iteration scheme. Here, it should be mentioned that most coupled problems are non-linear, even if all of the underlying sub-problems are linear (electrostatics-structure interaction, e. g.). Starting on the semi-discrete level and formulating the coupled problem as a block-structured system of algebraic equations or ordinary differential equations, its solution is in principle the same as the treatment of systems of non-linear equations [18], and the techniques mentioned above can be seen as generalized linear methods described in [18]. Furthermore, the application of modern minimization techniques for the solution of non-linear equations to the iteration procedures used for solving coupled problems may lead to an acceleration of those procedures [14]. Finally, time dependent coupled problems described by block-structured systems of ordinary differential equations or by differential algebraic ones can be treated with techniques developed for the parallel solution of systems of ordinary differential equations [7]. Those aspects and the integration of multilevel approaches into our coupled solution context will be in the centre of our future work.

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