Dynamic Electro-Thermal Simulation of Microsystems-a Review

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Abstract

An overview of electro-thermal modeling of microsystems is presented. We consider the most important coupling between thermal and electrical phenomena, and then focus on the industry's central concern, that of Joule heating. A description of different solution approaches for the heat transfer partial differential equation, which constitutes the central part of electro-thermal simulation, is given. We briefly review the analytical solutions and consider further the numerical approaches, which are based on spatial discretization of the thermal domain. Lastly, we describe the final level of approximation, the dynamic compact thermal modeling. We emphasize the formal model order reduction methods, because they directly follow the spatial discretization, and thus preserve the investment into the finite element modeling.

1. Introduction

Thermal management has become a crucial part of designing modern microelectronic and micro-electro-mechanical components and systems (MEMS). Only after a careful study of thermal effects in microsystems we can predict their performance, reliability and yield.

In integrated circuits, thermal management is important on all levels, starting from the transistor level [1], [2], over the chip level [3] - [5], the package level [6] - [8] and the printed circuit board (PCB) level [9], to the system level [10]. Self-heating of transistors changes their electric properties and this can affect the circuitry. High current during electrostatic discharge may increase the local temperature too much and destroy the transistor. Self-heating of interconnect

may reduce its average time to failure. It is important to position elements on a chip in such a way that the effect of heating is minimal in respect to the chip functioning. A package should be designed in such a way as to allow effective heat removal. Finally, the placement of semiconductor devices on PCB should also be optimal from the thermal management viewpoint. It is worthy of note that the reliability of the whole board is tied to its temperature regime because there are many mechanisms that lead to enhanced board degradation at elevated temperatures.

Numerous MEMS devices, such as thermal actuators [11], thermal flow sensors [12], microhotplate gas sensors [13], [14], tunable optical filters [15], [16] and many others are based on thermal effects. The heating changes optical properties in optical filters, reduces activation energies to allow metal oxides to detect gases and causes mechanical stress and thus movement in actuators. The heat transfer through the moving fluid allows us to measure the flow rate in heat-flow sensors.

All diverse engineering problems mentioned above have in common that an engineer should be able to predict the temperature distribution for the given electrical input and to estimate how the temperature in turn affects the electric part. In other words, he must run a joint electro-thermal simulation. As for the simulation of the electrical domain, there are usually already available tools, so the real task becomes to enhance them in order to take into account a variety of electro-thermal and thermo-electric effects. Hence, the solution of the heat transfer equation constitutes the central part of electro-thermal simulation.

Of course, in many cases the coupling of the heat transfer equation to other physical domains must be taken into account as well. Throughout this work, we will briefly review different cou-

plings and discuss what is necessary to decouple the heat transfer equation in order to be able to solve it separately.

Our main goal, however, is to make a unified description of different levels of solution approaches for the heat transfer partial differential equation.

Section 2 gives a short overview of different electro-thermal and thermo-electric effects in microsystems. The importance of the Joule heating effect for MEMS and microelectronic systems will be highlighted through examples in section 3. Sections 4 and 5 describe physical modeling with heat transfer equation and its possible couplings to other physical domains. Throughout section 6 we discuss how to solve the parabolic heat transfer equation on its own. The first topic is the linearization of the heat transfer equation, because the solution of the linear equation is much faster than that of the nonlinear one. The analytical solutions are briefly reviewed. We consider further the most frequent approach, which is based on spatial discretization of the thermal domain (often called the brute force method). The final level of approximation, dynamic compact thermal modeling (DCTM) is described in section 7. It allows us to effectively perform transient electro-thermal simulations on a system level. We include here the conventional, non automatic approaches such as RC-ladder network, semi automatic approaches such as modal approximation, as well as the increasingly popular model order reduction (MOR) approach, which can be made fully automatic. Lastly, section 8 concludes the review by displaying a schematics of discussed modeling approaches (see Fig. 12).

2. Overview of Coupled Electro-Thermal and Thermo-Electric Effects in Microsystems

A classification of the most important electro-thermal effects in semiconductor and IC-related materials utilized in microsystems is given in Table 1.1. A brief explanation of each effect is presented below (SI units are used).

	Thermal	Electrical
Thermal	heat conduction	thermoresistance Seebeck effect pyroelectricity
Electrical	**Joule heating** Peltier effect Thomson effect	electrical conduction

Table 1.1 Electro-thermal signal conversion effects in microsystems (see also [17]).

Heat conduction at the macroscopic level means that when a temperature gradient exists within a solid body, heat energy will flow from the region of high temperature to the region of low temperature. This phenomenon is described by Fourier's law:

$$q = -\kappa \nabla T \tag{1}$$

This equation determines the heat flux vector q (the amount of heat penetrating a unit of area per unit of time) in W/m^2 for a given temperature profile T and thermal conductivity κ of the body (a material property that describes the rate at which heat flows within a body for a given temperature difference) in W/(mK). All quantities relate to a specific point. The minus sign ensures that heat flows down the temperature gradient.

Electrical conduction describes the electrical current flow in the presence of the electrical potential gradient. If, in (1), the temperature is replaced by the electric potential φ and the heat flux vector by the electric current density vector $\boldsymbol{j}$, the solution of a corresponding problem of

electric conduction is given by:

$$\boldsymbol{j} = -\sigma \nabla \varphi \tag{2}$$

where σ is the specific electric conductivity in S/m.

Joule heating is the dominant mechanism for heat generation due to the flow of the electrical current through the material. It is defined by Joule's law, which in an ohmic conductor has the form:

$$Q = j^2 \rho \tag{3}$$

where j is the current density vector in A/m^2, ρ is the specific electric resistivity in Ωm and Q is the generated heat per unit volume in W/m^3. This is usually the main effect responsible for heat generation in resistively heated microsystems. A number of applications will be presented in section 3.

The thermoresistance effect states that the specific electric resistivity ρ of the material can be expressed as a function of temperature T:

$$\rho(T) = \rho_0(1 + \alpha T + \beta T^2 + \ldots) \tag{4}$$

where α and β are the temperature coefficients of the material in K^{-1} and K^{-2} respectively, and ρ_0 is the specific electric resistivity at the zero temperature. Positive temperature coefficients are peculiar to pure metals and some alloys. In a number of microsystem applications, metal resistors out of platinum, nickel, copper etc., are used as heating and sensing elements [13], [15]. In such cases (4) is on the one hand of paramount importance for temperature control, and on the other hand it contributes to the nonlinearity of the governing heat transfer equation via (3).

The Seebeck and Peltier effects are associated with a junction of two different conductors or semiconductors, a so-called thermocouple. If there is a maintained temperature difference between the junction and the free ends, an open-circuit Seebeck voltage is obtained at the non-connected end. The Seebeck effect is investigated for use in miniaturized voltage sources [18]. Those devices utilize heat generated by the human body and supply electronic devices (e.g. watches) with a minimum amount of electrical power. It is further used in thermoelectric infrared gas sensors [19]. The Peltier effect describes the generation or absorption (depending on the direction of the current) of heat in a thermocouple when the current flows through the junction in the absence of any temperature gradient. Contrary to Joule heating, the Peltier effect is reversible. It can be effectively used for heat transport opposite the temperature gradient and hence for cooling down the environment. It is mainly used for controlling the temperature of chips while measurements are being made. On-chip integrated Peltier elements are ideally suited for highly localized on-chip thermal stabilization [20].

The Thomson effect is complementary to the Peltier effect. In the Thomson effect two dissimilar materials are not needed but a current passed along a conductor, when a temperature gradient is maintained, results in either absorbance or generation of additional heat (in addition to Joule heat).

The pyroelectric effect describes the change of the electric polarization induced by a change of temperature in some nonlinear dielectric materials, such as PZT-ceramics, $PbTiO_3$, PVC etc. Pyroelectric materials are used within the thermal sensors and infrared detectors. Pyroelectric motion (infrared) sensors are used in a wide variety of applications. They are commonly found in security products, such as burglar alarms, motion detectors and intrusion detection systems

[21]. These sensors are also useful in environmental systems, lighting controls, visitor announcers, robotics, and artificial intelligence. They work by detecting the infrared heat emitted by the human body.

3. Joule Heating in Microsystems

Joule heating happens to be the dominant mechanism for heat generation in microsystems. Some devices like microsensors and microactuators are designed to optimize the Joule heating effect in a controlled manner in order to improve transduction efficiency. For the others, like integrated circuits (ICs), this effect is “parasitic“, and hence their design aims at the suppression of Joule heating. Below we review several MEMS devices whose working principle is directly or indirectly based on Joule heating and mention the most common “parasitic” effects based on Joule heating in microelectronic devices and their packaging.

Micro-hotplate-based devices, such as gas sensors [23] - [28], optical filters [15], thermal flow sensors [12], solid fuel microthrusters [29], thermal infra-red emitters [30] etc. use Joule heating to realize a desired functionality. Maximum temperatures for the operation of these devices obtain several hundred $^{\circ}C$. In order to significantly reduce the required electrical heating power, the resistive heater structures are placed on a thermally isolated micromachined platform called a membrane (see Fig. 1). Elevated temperatures may be essential for the onset of operation of the device (e.g. by gas sensors, microthrusters or infra-red emitters) or controlled temperate changes are used for tuning the structure‘s characteristics (e. g. for optical filters).

Micromechanical devices with electro-thermal actuation are used to perform direct mechanical actuation through thermal expansion resulting from Joule heating of selected

microstructures. Both in-plane actuators, based on thermally induced extension [33], and out-of-plane actuators [34], based on different thermal expansion coefficients that rely on the thermal expansion of silicon, polysilicon, nickel, or related materials have been extensively studied and used in MEMS structures. Thermal microactuators based on polymers such as polyimide, thermal bimorphs, pseudo-bimorphs, buckling beams, compliant structures and high-aspect-ratio structures have also been investigated (see [31] and the references there). The working principle of embedded electro-thermal-compliant actuator is shown in Fig. 2. The wide arms, which have lower electrical resistance than the narrow arms, draw more current and get hotter. As a result, the structure bends.

Microfluidic devices employ Joule heating to expel micro droplets out of micro fabricated reservoirs. In the reservoirs air-bubbles are generated within the liquid phase at the bottom of the reservoir that is above the heater, as schematically shown in Fig. 3. As the properties of micro-scale bubbles are dominated by surface tension effects, they tend to be very stable and hence useful for generating mechanical work. The dramatic increase in volume, which is due to bubble generation, forces small amounts of liquid to leave the chamber through a micro-nozzle. This technology is used in a broad spectrum of MEMS devices starting from ink jet print heads [35]. The thermopneumatic effect is further used to vaporize a working fluid through Joule heating. The increased gas pressure actuates a diaphragm. This deflection can be used in micropumps and microvalves [36] - [41] as components of micro-fluidic systems.

Microelectronic devices and their packaging are significantly influenced by temperature. In contrast to the previously described devices, Joule heating is not a desirable effect in microelectronic systems, but rather a “parasitic” one. Joule heating activates damaging mechanisms

such as corrosion of metallization and bond-pads, fatigue of wires or bonds, contact spiking, electrostatic discharge, electrical overstress (causing alone over 40% of all failure), electro-migration, thermal breakdown, wire bonded interconnections, flip-chip joints, cracking in plastic packaging etc. In addition to all of this there is almost no room for heat dissipation due to the huge number of transistors per unit area (modern VLSI contain 10^4 to 10^7 transistors per chip) and also no longer enough time due to higher frequency. Today‘s heat flux densities on the chip easily exceed 100W/cm^2 [43]. Not only the operating temperature itself, but also fluctuations are dangerous for the device’s reliability. It was already known in 1989 that a temperature oscillation of only 15 K increases the failure rate by eight times [43]. Due to the fact that temperature gradients are steeper in transient than in steady-state phase [45], transient (dynamic) thermal stresses are more dangerous. Violent operating conditions include the following dynamic effects: avalanche and electro-static discharge. Further effects such as temperature oscillations, current and voltage thermal drift or temperature gradient over the device [43], may degrade the device’s performance.

It should be noted that heat transfer modeling on its own varies in its importance for the above applications. In microhotplate-based devices it plays a major role and can be easily decoupled from other physical domains. In microfluidic devices, on the other hand, it plays a relatively small role, because it is strongly coupled to Navier-Stockes equations. In Fig. 4 the qualitative importance of heat transfer modeling for the different types of MEMS devices is schematically presented. However, it is difficult to set clear borders, because each engineering problem has to be considered on its own.

4. Physical Model - Heat Transfer Equation

The most general way to model heat transfer on the device level in crystalline semiconductors is the phonon Boltzmann transport equation. It describes the heat exchange between heat carriers (phonons), which are energy quanta of lattice vibrations [44] and the lattice. It should be used when the heat carrier's mean free path is comparable with the characteristic dimensions at microscale. To give an example, the phonon mean free path in Silicon at 300K is about 300nm. However, if one can assume that the Boltzmann-Maxwell distribution is valid for any small volume, or in other words that the temperature is defined at any point within the domain, a hyperbolic heat equation is used. It predicts a finite wave speed of heat propagation and is valued at very small time scale of femtosecond, for example during laser heating of thin metal films. If we further, assume that the speed of the thermal waves is infinite, the parabolic heat transfer equation can be used instead. Its solution is our main topic, since the assumptions mentioned above are valid for the devices in question, i. e. MEMS are approaching the limits, but don't reach them.

The parabolic heat transfer equation specifies the complete spatial and time profile of a temperature distribution within a computational domain Ω, limited by the boundary $\partial\Omega$. In solid it has a form:

$$\nabla\bullet(\kappa\nabla T) + Q - \rho C_p \frac{\partial T}{\partial t} = 0 \qquad (5)$$

where $\kappa(r)$ is the thermal conductivity in W/mK at the position *r*, $C_p(r)$ is the specific heat capacity (a material property that indicates the amount of energy a body stores for each degree increase in temperature, on a per unit mass basis) in J/kgK, $\rho(r)$ is the mass density in kg/m^3, $T(r, t)$ is the temperature distribution and $Q(r, t)$ is the heat generation rate per unit vol-

ume in W/m^3. (5) states that the temperature profile within a body depends upon the rate of its internally-generated heat, its capacity to store some of this heat by raising its temperature and its rate of thermal conduction to its boundaries (where the heat is transferred to the surrounding environment). The solution of (5) requires the determination of initial and boundary conditions (BC) for the simulation domain Ω. The temperature distribution T_0 at $t = 0$ serves as an initial condition:

$$\forall r \in \Omega \ , \ t = 0 \ , \quad T(r,t) = T_0(r) \tag{6}$$

Prescribed temperature distribution on the boundary in time can be modeled by **Dirichlet boundary condition** as follows:

$$\forall r \in \partial\Omega \ , \quad T(r) = T_{prescribed}(t) \tag{7}$$

Quite often, the boundary temperature is assumed to be constant and equal to the temperature of the surroundings and can be set to zero without the loss of generality.

Prescribed normal heat flux through the body boundaries $q_\perp$ in time can be modeled by **Neumann boundary condition** as follows:

$$\forall r \in \partial\Omega \ , q_\perp(r) = q_{prescribed}(t) \tag{8}$$

Convective heat transfer takes place when the whole subvolumes move from one place at a certain temperature to another at a different temperature. Hence, the convection is created by fluid flow. In many cases however, it is possible to eliminate the fluid flow from the computational domain by replacing it with a so-called **convection boundary condition**. It assumes that the normal heat flux through the boundary is proportional to the temperature difference between the boundary and the ambient temperature of the adjacent fluid:

$$\forall r \in \partial\Omega \ , \ q_{\perp}(r) \ = \ h(T - T_{ambient}) \tag{9}$$

where h is the heat transfer coefficient, which characterizes the thermal flow as well as the thermal contact between the conducting solid and adjacent fluid with temperature $T_{ambient}$. Again, quite often $T_{ambient} \ = \ 0$. It should be noted that the convection boundary condition turns into Neumann for $h \ = \ 0$, or into Dirichlet for $h \to \infty$.

Heat radiation mechanism can be modeled by so called **radiation boundary condition** as follows:

$$\forall r \in \partial\Omega, \ q_{emitted}(\boldsymbol{r}) \ = \ \varepsilon \cdot \sigma \cdot A(T^4_{surface} - T^4_{ambient}) \tag{10}$$

where $q_{emitted}$ is the emitted heat transfer rate (power), ε is the surface incivility, σ is the Stefan-Boltzmann constant ($5.669 \cdot 10^{-8}$ W/m^{2}K^4) and A is the radiation surface.

It is worthy of note that in practice it is important to be able to solve (5) with different boundary conditions, that is, to create a boundary conditions independent (BCI) model [62]. This is possible at the level of detailed solution of (5) (see section 6.3) but is difficult at the level of compact models (see section 7.1).

5. Coupling of Heat Transfer Equation to Other Physical Domains

In the general case, the heat transfer equation (5) is coupled with other partial differential equations already at the device level. Let us consider the most important coupling and discuss what approximations are necessary to decouple the equations in order to be able to efficiently solve (5) on its own.

The first coupling comes through the environment, since the device is usually surrounded by moving fluid (either gas or liquid), which serves to remove heat by natural or forced convec-

tion. The heat transfer in the moving fluid is generally a part of the solution of Navier-Stokes equations. They can be coupled with (5) in order to describe the overall heat transfer, which makes the resulting set of equations quite complicated. In some cases it is possible to decouple them by applying the convection boundary condition (9).

If there is a convective flow with specified flow velocity $\vec{v}$ within a computational domain, the heat transfer equation (5) gains additional, so-called "thermal flow term" $\rho C_p \vec{v} \nabla T$. This term complicates the analytical solutions. However, numerical methods for solving (5) can treat the thermal flow term with small additional effort and moreover MOR-based solutions can be used as well [46].

If the flow velocity within a computational domain cannot be specified, as in the extreme case of bubbles formation by microfluidic devices for example, there is no way of decoupling the (5) from Navier-Stokes equations. Hence, the solution of spatially discretized coupled system becomes costly.

In the case of thermo-mechanical coupling, a good approximation is the solution of the thermal problem on the Lagrangian grid [47]. Then, it is possible to solve the thermal problem on its own and to use the temperature distribution to estimate additional stress, which is due to thermal expansion.

The electro-thermal coupling is present through the heat generation rate Q, emerging mostly from the Joule effect (3). In general, in order to solve for the current in (3), it is necessary to solve the Poisson equation, which (in the case of an isotropic resistive heater which is free from electrical charges) has a form:

$$\nabla \bullet j = \nabla \bullet (\sigma \nabla \varphi) = 0 \tag{11}$$

It is possible to solve the Poisson equation for the unknown electric potential field, provided that the geometry of the heater, its specific conductivity and the boundary conditions are specified [22]. Note that (11) depends only implicitly on time, due to possible changes in boundary values or changes in conductivity. This is because the speed of the electron propagation is very high. We assume that (11) holds instantly at any given time. It should be noted that if the electrical current frequency reaches the kHz range, i.e. when capacitance and inductive effects have to be accounted for, a higher level model based on the solution of the electromagnetic Maxwell equations is required.

By inserting (11) into (3) the heat generation rate within an ohmic conductor changes into:

$$Q = \frac{j^2}{\sigma} = \sigma \cdot (\nabla \varphi)^2 \tag{12}$$

By assuming homogeneous heat generation over a lumped resistor (12) simplifies to the well known:

$$Q = I^2 R = \frac{U^2}{R} \tag{13}$$

where I is the current passing the lumped resistor, due to potential difference U over it, R is its resistivity and Q is the total heat generated within the resistor's volume. By replacing Q in (5) with (13) the coupling to the Poisson equation is avoided. However, (13) may not offer a good approximation in all cases. For example if resistors with complex geometries are present, homogeneous heat generation can be hardly assumed and in this case the consistent electro-thermal simulation is needed (that is a simultaneous solution of (12) and (5)), as shown in Fig. 5.

The electro-thermal coupling at the system level (with assuming a homogeneous heat generation within a lumped heater) for the special case of resistively heated microdevices, is schematically presented in Fig. 6. Note that coupling becomes more complicated in case of ICs, i. e. when the temperature impact on semiconductor devices is taken into account [50].

A spatial discretisation of (5) over the complete simulation domain (e.g., the whole chip) is necessary in order to obtain a thermal system shown in Fig. 6:

$$C\dot{T} + KT = F \cdot Q \tag{14}$$

where C and K are the global heat capacity and heat conductivity matrices, $T(t)$ is the temperature vector, F is the load vector (matrix) and $Q(t)$ is the heat source vector. Obviously, in order to effectively perform a system level simulation, it is necessary to keep the dimension of (14) as moderate as possible. This is exactly the goal of compact modeling described in chapter 7.

6. Solving the Heat Transfer Partial Differential Equation

In the following as a border between analytical and numerical solutions of (5) we will use the discretization of the computational domain in space, which necessarily leads to an ordinary differential equation system. One can start with a set of functions in the computational domain $f_i(x, y, z)$ for the infinite series expansion and then proceed systematically to determine the unknown coefficients $a_i(t)$ within the series in order to solve the heat transfer equation. The separation of variables method gives:

$$T(x, y, z, t) = \sum_{i=0}^{\infty} a_i(t) f_i(x, y, z) \tag{15}$$

In general if the expansion functions a_i and f_i exactly satisfy the BCs for the problem, we refer to a solution as analytical. An alternative is to split the domain into many small pieces, that is to discretize it in the space. Then one can approximate the temperature field within an element by using local shape functions and express the whole temperature field in a piece-wise fashion. In this case, we refer to a solution as numerical.

6.1 Linearization

When material properties in the heat transfer equation are constant, it is called linear. In this case, there are many mathematical benefits, for example one can use the superposition principle. Computationally it is definitely much easier to solve a linear partial differential equation. Almost all analytical solutions require the heat transfer equation to be linear. For numerical methods this is not required but it is no doubt advantageous to do so if possible. In general, however, the material properties are temperature dependent and (5) has a form:

$$\nabla\bullet(\kappa(T)\nabla T) + Q - \rho C_p(T)\frac{\partial}{\partial t}(T) = 0 \tag{16}$$

It is always possible to perform linearization around the operation point (temperature) in order to convert a non-linear heat transfer equation to a linear one. After obtaining a set of linear models around a chosen set of temperatures in this way, one can use a sort of weighting function, as done in [48] to e. g. extract a non-linear compact thermal model.

In some special cases it is further possible to use certain transformations that linearize (5). Under the assumptions that only the thermal conductivity κ is temperature dependent and that

κ is not a function of space, the authors in [49] suggest using the Kirchoff transformation of the form:

$$\theta = T_s + \frac{1}{\kappa_s}\int_{T_s}^{T} \kappa(T)dT \tag{17}$$

where $\kappa_s = \kappa(T_s)$ and T_s is the heat sink temperature, which fully linearizes a static part of (16). By additionally defining a new time variable, τ:

$$k_s\tau = \int_0^t k(\theta)dt \tag{18}$$

where diffusitivity $k_s = \kappa_s / \rho C_p$, the time-dependent non-linear heat transfer equation (16) becomes fully linearized:

$$\nabla^2\theta + \frac{Q}{\kappa_s} - \frac{1}{k_s}\frac{\partial\theta}{\partial\tau} = 0 \tag{19}$$

6.2 Analytical Solutions

Most published analytical solutions assume a simple geometry of the computational domain. Examples are the thin rectangular heat source or a volume heat source on the top of an infinite medium. The latter is often used for modeling a bipolar transistor (see [50] and the references there). Another example is a stacked layer structure that can be infinitely extended in length and with directions, used for modeling a power FET transistor [51]. The most general analytical solution so far is based on [49], in which a linearized heat conduction equation (2.22) is analytically solved in the rectangular (multilayer) thermal domain with arbitrarily distributed volume heat sources. It is in principle possible to divide a region with arbitrary geometry into

rectangular thermal subvolumes and to apply the solution from [49]. However, in this case the problem of coupling these subvolumes must be solved as well (this is still not possible).

Different analytical approaches use Green functions [52], [50], Fourier series [49], [53] or Fourier transform [51].

As a conclusion to this subsection we want to state that although the analytical solutions require lower computational effort and are preferred by microsystem designers in the above-mentioned special cases, it is difficult to use them in general.

6.3 Numerical Methods

There are several methods associated with a mesh, which partitions the arbitrary computational domain into smaller units. These are the finite difference method (FDM), the finite volume method (FVM), the finite element method (FEM) and the boundary element method (BEM). They semi-discretize the heat transfer partial differential equation (5) and transform it into a system of ordinary differential equations (14). An overview of these methods and a discussion of similarities and differences between them can be found in [54]. For the heat transfer equation (5), a transmission line matrix (TLM) approach can be used as well [55], [56]. This approach represents a physical model of heat flow as a sequence of voltage (temperature) pulses traveling through a matrix network of transmission lines. This method requires a rectangular mesh and a creation of an RC network.

Lastly, each spatial discretization can be transformed into an equivalent thermal RC network. In this subsection we will briefly discuss the resemblance of thermal and electrical circuits.

We have mentioned the importance of creating a boundary conditions independent model. Let

us briefly explain, how a typical commercial solver generates such a model. The first step is the "pure" discretization of the computational domain without having specified the heat generation rate or boundary conditions. It results in two system matrices, C_{BCI} and K_{BCI}, which are stored in the software database. In the general case, these matrices depend on temperature and are not formed explicitly but rather are stored as a list of element matrices. Both are sparse and C_{BCI} is quite often lumped, which means that it is converted into a diagonal matrix. The dimension of C_{BCI} and K_{BCI} equals the number of the introduced finite element nodes. We refer to this matrices as BCI, because it is possible to apply boundary conditions to a model described with C_{BCI} and K_{BCI} without repeated discretization.

After the Neumann and convection boundary conditions have been introduced, a system of ordinary differential equations is written as:

$$C_{BCI}\dot{T} + K_{BCI}T + \sum K_{con}T = \sum f_{source} + \sum f_{Neumann} + \sum f_{con} \tag{20}$$

where the sum contains all the heat sources and boundary conditions. The volume heat sources and the Neumann boundary conditions contribute only to the load vector, while the convection boundary conditions contribute to both the load vector and the heat conductivity matrix. It is possible to add the scaling factors to each heat source and boundary condition. Hence, the equation (20) can describe various external conditions without further need for any changes.

The use of Dirichlet boundary conditions, however, changes (20) as follows:

$$C\dot{T} + KT = \sum f_{source} + \sum f_{Neumann} + \sum f_{con} + \sum f_{Dirichlet} \tag{21}$$

where the dimension of all vectors and matrices is reduced by the number of nodes to which the constant temperature is applied (Dirichlet nodes). C and K are obtained from C_{BCI} and K_{BCI} by crossing out those columns and rows which belong to the Dirichlet nodes. However,

the use of Dirichlet boundary conditions makes (21) less flexible, as it is impossible to replace them with different boundary conditions when once applied. In (20), one can change BCs by simply using zero scaling factors. Luckily, one can always replace the Dirichlet boundary conditions with the convection BCs if a very high value for the film coefficient is used.

Equations (20) and (21) are equivalent to (14) and can be directly plugged into the electric simulator as an equivalent RC-network. In order to highlight a resemblance of thermal and electrical circuits, let us observe a parallel RC circuit in Fig. 7.

It is described by:

$$C\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}\begin{bmatrix} \dot{V}_1 \\ \dot{V}_2 \end{bmatrix} + \frac{1}{R}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}\begin{bmatrix} V_1 \\ V_2 \end{bmatrix} = \begin{bmatrix} I_1 \\ I_2 \end{bmatrix} \tag{22}$$

When comparing (22) with (14) it is easy to see that the heat capacity matrix can be released by capacitor elements, the heat conductivity matrix by resistor elements and the heat source vector (matrix) by current sources. The equivalent thermal networks were derived for different types of finite elements [60]. Fig. 8 shows a conductive thermal network for a tetrahedral element with a convective boundary.

It should be noted that the transformation of (14) into an equivalent thermal RC network is exact, i. e. no approximation (in the sense of compacting the circuit) is made so far.

Additional to transforming (14) into an equivalent thermal RC network, it can also be implemented in equation form in hardware description language (HDL) directly. Some examples of implementations for electro-thermal modeling of power electronic circuits and multiple domain devices in VHDL can be found in [57]-[59]. The major problem, however, is the com-

putational efficiency, that is, the size of a thermal problem (see next section).

7. Dynamic Compact Thermal Modeling

As already mentioned, it is the dimension of (14) which makes the simulation time-consuming. For a variety of MEMS devices the order of the resulting thermal ordinary differential equation system exceeds 100,000. Hence, it is prohibitive to use these models during system-level simulation. Instead, accurate dynamic compact thermal models (DCTM) are required. The methods for constructing DCTM can be divided into three general groups: non-automatic methods such as different RC ladder network approaches, semi-automatic methods such as modal approaches and model order reduction methods which can be made fully automatic.

7.1 RC Ladder Approach

A large number of DCTM approaches are based on fitting an RC ladder network on the observed (measured or numerically computed) system response, using a suitable optimization technique. In this case, however, the RC ladder network is based on an attempt to lump a distributed thermal domain. For 1D heat conduction, if we subdivide the domain into a large number of small slabs whose thicknesses L go to zero, we get a so-called Cauer ladder network (see Fig. 9 left) with grounded capacitors and floating resistors. This can be transformed into a Foster network (Fig. 9 right) via standard circuit transformation algorithms. While the Cauer network appears to be a small version of the large equivalent circuit described in the previous section (that is a fine mesh was replaced by a coarse one), the Foster network has no physical meaning. In both cases, the question is how to set a proper number of RC pairs or, in the case of 2D and 3D thermal conduction, how to choose a proper network structure at all.

In [61] the authors suggest a robust method based on computing a time-constant spectrum

function connected to Foster network. A Foster network representation brings along an infinite number of time-constants (each R_iC_i pair represents a time constant $\tau_i = C_i \cdot R_i$) and so defines a continuous τ spectrum. The step response of a single R_iC_i stage is $R_i(1 - exp(-t/\tau_i))$. Hence, the unit-step response of the Forster network can be constructed as a sum of these exponential terms:

$$T(t) = \sum_i R_i(1 - exp(-t/\tau_i)) \tag{23}$$

After replacing R_i with a continuous spectrum, the above sum can be replaced by the integral over the whole τ range:

$$T(t) = \int_{-\infty}^{\infty} R(\xi)(1 - exp(-t/exp(\xi)))d\xi \tag{24}$$

where $R(\xi)$ is the time-constant spectrum function defined on the $z = ln(t)$ and $\xi = ln(\tau)$, logarithmic time axes. Lastly, the relationship between $T(t)$ and spectrum can be expressed by convolution as:

$$\frac{d}{dz}T(z) = R(z) \otimes w(z) \tag{25}$$

where $w(z) = exp(z - exp(z))$. Hence, from the measured step response T(t) we can discretize to determine a suitable number of RC ladder elements in the Foster circuit required to represent a (preferably multilayer) system prior to fitting. As the Foster network has no physical meaning, it has become an engineering practice to convert it back to Cauer form. This method also works for the 2D and 3D heat conduction, but is unfortunately applicable only to single conduction path, i. e., to single-input-single-output (SISO) problems.

For the multiple-input-multiple-output (MIMO) problems, not only the number but also the structure of a compact RC ladder network must be specified. Recently, the authors

in [41] have suggested the application of evolutionary algorithms for setting the correct topology of the compact model.

Special challenge in dynamic compact thermal modeling, is to construct a boundary condition independent compact model, which would be reusable for different surroundings. This means that if e. g., a chip producer does not know the conditions under which the chip will be used, the compact thermal model must allow an engineer to research how the environmental changes influence the chip temperature. The two European projects, DELHPI and PROFIT have addressed the need to produce an accurate and boundary condition independent compact thermal models of a chip [62] - [66], which would simplify the chip cooling simulation of coupled thermal and fluidic domain. The chip benchmarks representing boundary condition independent requirements are described in [67]. Related discussions can be also found in [68] and [69]. The goal of the PROFIT project was to extend the methodology to transient compact thermal models by using methods from [61] and [70]. The current solutions from both projects are mainly based on data fitting for the apriori chosen resistor network.

In spite of the large number of related methods suggested in the last years (an extensive review can be found in [71]), the RC network extraction remains a non-automatic approach, which requires a designer to choose the correct number and position of the RC ladders without strict guidelines and to perform a time-consuming parametrization.

7.2 Modal Approaches

It is well-known from structural mechanics that an elastic string vibration under the action of arbitrary external force, can be viewed as a linear combination of different vibrating modes, each one corresponding to a resonance of the string. Although their number is infinite, the

actual response can be approximated quite well by considering only the few first harmonics. This is how the elastic string, which is a distributed system can be compacted into a lumped system with only a few degrees of freedom. In terms of the partial differential equation governing a string vibration this means that one has to compute the eigenvalues, which are the vibration frequencies, and the eigenfunctions, which are the spatial forms of vibrations for each mode. Out of the first few eigenfunctions a compact model can be constructed.

In an analog manner, the temperature can be expressed as series expansion around a set of "dominant" eigenfunctions U_j:

$$T(r,t) \cong \sum_{j=1}^{k} U_j(r) \cdot V_j(t) \tag{26}$$

where V_j are jet unknown expansion coefficients. By substituting (26) into (5), multiplying it by V_i and integrating, it is possible to get a reduced model [71] of the form:

$$C^* dV(t)/(dt) + K^* V(t) = s(t) \tag{27}$$

where $C^*_{ij} = \int \rho C_p U_i U_j dr$, $K^*_{ij} = \int U_i \nabla(\kappa \nabla U_j) dr$, $s_i = \int U_i Q dr$, $i, j \in [1, k]$.

Unfortunately, the analytical solution of the eigenvalues problem for heat conduction partial differential equation (5) is available only for some simple geometries [72]. Hence, a first approximation is to perform spatial discretization and to compute the eigenvalues and corresponding eigenvectors of the system matrix of (14). To do this, we need to reduce (14) to a single matrix representation as:

$$A\dot{T} = T + Bu(t) \tag{28}$$

where $A = -K^{-1}C$ and $B = -K^{-1}FQ$. The number of eigenvectors of A equals the number n of finite element nodes. It is possible to reduce a system (28) by projection, whereas a projection matrix $V_{modal} \in C^{n \times r}$ is composed of r eigenvectors of A. Now the n-dimensional equation (28) can be projected onto r-dimensional subspace as follows:

$$V_{modal}^{T} \cdot A \cdot V_{modal} \cdot \dot{T}_r = V_{modal}^{T} \cdot V_{modal} \cdot T_r + V_{modal}^{T} \cdot Bu(t) \tag{29}$$

where T_r is a generalized variable vector. The question which remains is how to choose the "dominant" modes (eigenvectors). For the defined thermal output $y(t) = E^{T} \cdot T$ (E is either a vector or matrix), one can observe the transfer function $G(s) = E^{T}(sI - A)^{-1}B$, and choose those poles (and associated eigenvalues) which are around the region of frequencies of interest. Nevertheless, the choice of important modes still requires the designer's action, which makes a modal approach manual.

7.3 Model Order Reduction

The only group of DCTM methods which can be made fully automatic, i. e. only with the minimal intervention by the designer, are the formal mathematical model order reduction (MOR) methods. Hence, among microelectronic and MEMS designers they are becoming increasingly popular [73] - [93].

The ideas of mathematical model order reduction have been developed in the control theory and are applicable to first order linear ODE systems, such as (14). The development of model reduction of non-linear systems is still in its early stages [94], [33]. According to the control theory, (14) should be written in the right-hand side state-space formulation as:

$$\begin{aligned} \dot{T} &= AT + Bu(t) \\ y(t) &= E^T \cdot T \end{aligned} \tag{30}$$

where the system is treated as a black box, i. e. the internal state vector of temperatures $T \in R^n$ is not directly accessible to an external observer. The controller can influence the system state through the input functions specified by the vector $u(t) \in R^m$ and distributed to the internal nodes in accordance to the input matrix $B \in R^{n \times m}$. As the number of inputs is typically small $m \ll n$, the matrix B has a small number of columns. Furthermore, the observer is interested in only a few outputs, specified by the vector $y \in R^p$. The required outputs are selected from the complete state vector via output matrix $E \in R^{n \times p}$. Hence, a high-dimensional ODE system, governed by a small number of external inputs, has to be solved in order to determine a small number of relevant outputs.

Let us also mention at this place the all-important transfer function of the system (30), defined as:

$$G(s) = E^T (sI - A)^{-1} B \tag{31}$$

where s is the laplace variable and I is a unity matrix of the dimension n. Although $G(s)$ is a relatively small matrix with p rows and m columns, its computation requires the inverse of a large-scale system matrix A.

While searching for a possibility to reduce the number of state variables, i. e. equations in (30), let us transform the state vector T using a transformation matrix $V_n \in R^{n \times n}$ as follows:

$$T = V_n \cdot z \tag{32}$$

Hereby z is the new state vector in terms of generalized coordinates expressed by the transformation matrix. It is important to understand that if T has the spatial and physical meaning as a

vector of temperatures belonging to FE nodes, z has none of either. Rather, it is a vector of multiplication factors for the "global shape functions" given by the columns of matrix V_n.

To make this more clear, let us take a closer look at discretization methods where the temperature over the whole domain is approximated as a piece-wise linear combination over the elements:

$$T(r) = \sum_{\Omega_1}^{i=1,n} c_i^1 N_i^1(r) + \ldots + \sum_{\Omega_e}^{i=1,n} c_i^e N_i^e(r) \tag{33}$$

where n is the number of free coefficients c_i in each element (these can be the nodes temperatures for example) and e is the total number of elements. A property of each local shape function N_i is that its value is one at the i-th node and zero outside the finite element. Within the element it can linearly decay between one and zero. The only way to directly reduce a system based on (33) is to coarsen the mesh, i. e. to chose the shape functions which cover several elements. This, however, results in a significant lost of precision (see Fig. 10 top).

On the other hand, each column of matrix V_n in (32) can be seen as a linear combination of the local shape functions, i.e. as a global shape function over the whole heat transfer domain. This gives hope that it may be possible to truncate some of the generalized coordinates z and therefore reduce a dimension of the system (32) without losing much accuracy (see Fig. 10 bottom).

Both ways of compressing information which are shown in Fig. 10 have their advantages and disadvantages. By coarsening the mesh, one preserves the physical nodes, but looses the precision. By performing mathematical model order reduction, one looses the physical nodes, but preserves accuracy (as will be explained below). Note that those two methods do not exclude each other, but can rather be combined in order to maximally increase the efficiency.

Let us emphasize that after the transformation, equation (30) changes to:

$$\begin{aligned} \dot{z} &= W_n^T A V_n \cdot z + W_n^T B u(t) \\ y(t) &= E^T V_n \cdot z \end{aligned} \tag{34}$$

where $W_n, V_n \in R^{n \times n}$ are biorthigonal, which means that $W_n{}^T \cdot V_n = I$. For the external observer (34) behaves exactly the same way as (30), i. e. one can easily prove that the transfer function (31) does not change.

As already mentioned, model reduction is based on the idea that one can find such a transformation when one can accurately represent the state vector with just a few generalized coordinates. In other words, a transformation exists when one can truncate most of the generalized coordinates, that is to approximate:

$$T = \left[V_r \; V_{n-r} \right] \cdot \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \tag{35}$$

through

$$T = V_r \cdot z_1 + \varepsilon \tag{36}$$

with the error vector ε being small. This, on the other hand, changes (34) to a low dimensional system:

$$\begin{aligned} \dot{z_1} &= A_r z_1 + B_r u(t) \\ y_r(t) &= E_r^T \cdot z_1 \end{aligned} \tag{37}$$

with $A_r = W_r^T A V_r$, $B_r = W_r^T B$, $E_r = V_r^T E$ and $W_r^T \cdot V_r = I$. The number of inputs and outputs in (37) is the same as in (30), whereas the number of equations (dimension of the state vector) is smaller. This transformation is schematically shown in Fig. 11.

The equation (36) can be also seen as a projection of a *n*-dimensional state vector to a *r*-dimensional subspace $r \ll n$, defined by the columns of matrix V_r. (37) is a projection of the whole system (30). The output of the reduced system is, however, not the same as that of (30) or (34), since we have introduced the truncation error ε. The goal of model order reduction is to minimize this error either in the time domain $min\|y(t) - y_r(t)\|$ or in the Laplace domain $min\|G(s) - G_r(s)\|$, where the transfer function $G_r(s)$ of the reduced system is defined as:

$$G_r(s) = E_r^T (sI - A_r)^{-1} B_r \tag{38}$$

There are several model reduction methods for linear ODE systems which produce small ε. They take the system matrices *A* and *B* of the linear system as input and perform linear algebra manipulations with them in a different manner to construct W_r and V_r. Let us emphasize that, unlike the non-automatic RC-ladder approach, there is no explicit minimization procedure for ε and in a way, one obtains the best topology of a reduced system simultaneously with its system matrices. These methods and their most important properties are summarized in Table 1.2.

	Advantages	Disadvantages
SVD-based (Balanced Truncation Approximation, Singular Perturbation Approximation, Hankel Norm Approximation)	have a global error estimate, can be used in a fully automatic manner	computational complexity is $O(n^3)$, hence can be used only for systems with less than a few thousand unknowns
SVD-Krylov (low-rank Grammian approximants) and matrix sign function methods	have a global error estimate and the computational complexity is less than $O(n^2)$	currently under development
Padé approximants (moment matching) via Krylov subspaces by means of either the Arnoldi or Lancsoz algorithm	computationally very advantageous, can be applied to very high-dimensional 1st order linear systems	do not have a global error estimate. Hence, it is necessary to select the order of the reduced system manually

Table 1.2 Methods for model order reduction of linear dynamic systems.

The most advanced MOR methods are established by control theory, which allows us to make the strong statement that model reduction of a linear dynamic system is solved in principle. The control theory methods [97] are based on singular value decomposition (SVD) and offer guaranteed error bounds for the difference between the transfer function of the original high-dimensional and reduced low-dimensional system. Model reduction based on these methods can be made fully automatic. A user merely has to set an error bound, and then the algorithm will find the smallest possible dimension of the reduced system which satisfies that bound. Alternatively, a user specifies the required dimension of the reduced system and then the algorithm estimates the error bound for the reduced system. Unfortunately, the computational complexity of current implementations is of order $O(n^3)$, with n the order of the large system of ODEs. In other words, even though the theory is valid for all linear dynamic systems, practically we can use it for small systems only. The SVD-Krylov methods, based on low-rank Grammian approximants [98]-[101], and the matrix sign function methods [102] have resulted from the efforts to find computationally effective strategies in order to apply control theory methods to large-scale systems. However, they are currently under development and we will have to wait for the experience to grow in this field. Most of the practical work in model reduction of large linear dynamic systems has been tied to Padé approximants (so-called moment matching) of the transfer function via Krylov subspaces [103], [104] by means of either the Arnoldi or the Lanczos process. In the literature, there are some spectacular examples where, using these techniques, the dimension of a system of ordinary differential equations was reduced by several orders of magnitude, with minimal lost of precision. The disadvantage is that Padé approximants do not have a global error estimate, and hence it is necessary to select the order of the reduced system manually [105]. Some engineering approaches on how to auto-

matically estimate the reduction error are given in [106].

Numerical results for small systems show that Hankel singular values (system properties, which reflect the contributions of different entries of the state vector to system responses [108], [109]) decay very fast for the discretized heat transfer equation (see [107] and [110]). This can be viewed as an empirical proof that just a few global functions are enough to accurately solve the heat transfer problem and the only question is how to find them, i. e., how to define matrix V_r.

Model order reduction based on the Arnoldi algorithm, on the other hand, allows us to restore the whole domain. In a way, it can be viewed as a fast integration procedure.

Finally, let us get back to the physical sense of the internal nodes in the reduced models. The goal is to approximate the original system, which means the smaller error, the more physical sense. If we think of RC parameters as the amplitudes for global functions, then any network, including the Foster RC-network, has a valid physical sense for thermal modeling.

However, conventional model reduction fails to preserve parameters during model reduction process. This limits severely its applicability for the creation of boundary condition independent reduced models or for the design flow and system level simulation. In our knowledge, the first work on parametric model reduction has been presented by Weile at al [76] in 1999 and applied to describe frequency depended surfaces in [77]. This approach has been generalized from two to many parameters in [78] and in parallel re-discovered in [79]-[81]. An empirical solution to a similar problem has been suggested in [82] and an alternative algorithm in [83]. Note that different authors use different names for the same method: multiparameter model reduction in [78], multidimensional model reduction in [79] and [80] and multivariate model

reduction in [81]. We refer to parametric model order reduction. In [81][83][84], this approach has been successfully applied to a thermal problem when film coefficients have been preserved as symbols in a reduced model.

In case when the material properties in the heat transfer equation must be kept as temperature dependant and linearization is not possible, one can use nonlinear model order reduction. The wide spread approach here is a proper orthogonal decomposition (POD) which is also known as Karhunen-Loéve transformation [85]. In POD, in order to find an appropriate low-dimensional subspace (36), one uses the results of the full order simulation of the original dynamic system (30). The first step is to perform one or more simulations of the full model and to collect a series of so-called snapshots of temperature distributions $T(t_i)$ which correspond to different simulation times t_i of (30). This is the main disadvantage with respect to linear systems, where the model reduction process is based on the system matrices only, i. e. without performing a full model simulation. Furthermore, for linear systems, it was possible to perform model reduction for any input function, whereas for nonlinear systems it is necessary to choose the most typical input functions and a reduced model depends on them. Unfortunately, there exist no formal rules on how to choose the number of snapshots or at what times they should be taken. Nevertheless, there are already examples of successful application of POD to thermal [86], [87] and coupled-domain MEMS models [88]. The most recent development in nonlinear model order reduction is the trajectory piecewise-linear MOR technique [89] which is based on Arnoldi algorithm and the weighted combination of the linearized macromodels at different linearization points. It has been recently applied to heat-transfer macromodeling of MEMS [33].

8. Discussion and conclusion

In this review we have highlighted the importance of heat transfer modeling, which is presently a central part of the electro-thermal simulation of microsystems. We have discussed in which cases it is possible to decouple the heat transfer partial differential equation from other physical domains, in order to be able to solve it separately. Unfortunately, analytical solutions are only available for simple geometries, whereas either approximations or numerical methods must be used for complex geometries.

However, the numerical solution of the heat transfer PDE via e. g. finite elements is often impractical or even prohibitive if we want to simulate the whole system with a large number of interconnected devices. Again, the number of resulting ordinary differential equations for a single device easily exceeds 100,000. Even by using a domain decomposition technique on parallel computers, this huge number of unknowns demands large resources of CPU-time and memory. Hence, a reduction of the number of unknowns to a lower-dimensional system, known as dynamic compact thermal modeling has become a standard for microsystem simulation. We recommend a DCTM via model order reduction, because it presently offers an accurate and effective solution for microsystems and enables an automatic system-level modeling. A schematics of the discussed and recommended researched paths is shown in Fig. 12.

To this end, we have presented the conventional, non automatic approaches (RC-ladder network), semi automatic approaches (modal approximation), and the increasingly popular model order reduction approaches, which can be made fully automatic. However, they all consider the DCTM of a single device only. Since microelectronic and MEMS are usually composed of subsystems that are interconnect to array structures for example, it is desirable, especially for a

large number of subsystems, to extract a heat-transfer macromodel of each subsystem on its own and then to couple them back together. Some works on this topic can be found in [111] - [113].

At the end of this review, we would like to highlight the possibility of solving the so-called inverse problem by model order reduction. Often, it happens that a MEMS designer has the measured data, but is uncertain about the material parameters (for example the heat capacity and thermal conductivity of thin film materials, which strongly depend on fabrication conditions). In such a case, it is possible to use model order reduction within a fast design alteration cycle (see Fig. 13) to extract the true parameter values via optimization. Fig. 13 shows that MOR allows the change of the input function on the level of compact model. It further allows a quick design change without a time-consuming recomputation of the full model. For example, if we change material parameters, we have to built a new finite element model. Luckily, due to MOR we are able to avoid its slow recomputation, and can work with reduced model instead. However, the main goal of the future research should be a parametric model order reduction which would allow major design changes solely within a reduced model.

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Captions for figures

Fig. 1 Photomicrograph of a single microhotplate element from [31].

Fig. 2 An example of electro-thermal embedded actuation: (a) original configuration; (b) deformed configuration superimposed on the original. From [32].

Fig. 3 Functioning principle of a thermopneumatic microvalve from [42].

Fig. 4 Qualitative importance of heat transfer modeling for different types of MEMS devices.

Fig. 5 Sequence of the coupled electro-thermal simulation.

Fig. 6 Schematics of coupled electro-thermal simulation at system level for the resistively heated microsystems. Homogeneous heat generation is assumed.

Fig. 7 A parallel RC circuit.

Fig. 8 Thermal impendance network for a tetrahedral element for use away from the boundaries, from [60].

Fig. 9 Cauer RC ladder network (left) and Foster network (right).

Fig. 10 Order reduction via coarsening the mesh (top, from [95]) and via truncating the generalized coordinates (bottom, from [96]).

Fig. 11 Schematics of the system before and after model reduction step.

Fig. 12 Schematics of discussed and recommended (bold) research paths in electro-thermal modeling of microsystems.

Fig. 13 Application of MOR to parameter extraction in MEMS design process.