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Transient electro-thermal simulation of microsystems with space-continuous thermal models in an analogue behavioural simulator

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Abstract

In many microsystems (MEMS), thermal effects have significant importance and system-level electro-thermal simulation is needed to shorten the product development cycle and to increase system reliability. The possibilities for space-continuous simulation of electro-thermal problems using an analogue simulator and an analogue hardware description language are described. In comparison to commercial finite element simulators, the relative error of thermal simulation is $<0.08\%$ for three-dimensional static analyses. Transient thermal problems with coupled electronic components are simulated. © 2000 Published by Elsevier Science Ltd. All rights reserved.

1. Introduction

MEMS (microsystems) are miniaturized devices with several important differences in comparison to macroscopic objects. Firstly, the volume and mass are small (proportional to the cube of the object size), so inertial or magnetic forces may be neglected in many applications. However, the surface area decreases proportionally to the square of the object size, so surface forces (electrostatic, electromagnetic, pressure) are of greater significance for the functionality of a microdevice than for its macroscopic counterpart. Due to various technological limitations, the parts of the microsystem are shaped in simple forms such as beams, bridges and membranes. However, recent advances in fabrication technology, have led to less conservative design methodologies, that is, using arbitrary 3D shapes.

As a result of the miniaturization and the integration of microelectronics and MEMS, thermal effects contain higher energy densities and cover a wider frequency range. In opposite to monolithic ICs, dissipating devices can be located anywhere in the volume. The neighbouring components in a microsystem device are mutually influenced by thermal flows, but also other closely coupled physical fields can influence a system-level behaviour of the device. Such bi-directional multi-domain interconnections are difficult to simulate with standard simulation environments. In various microsystems, the thermal process is exploited

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as an actuating principle [1,2]. On the other hand, many researchers have reported devices with parasitic thermal behaviour that needs to be analysed. Some of the problems have been described in Ref. [3]. In order to achieve shorter design cycles of complex microsystems, an easy-to-use and flexible electro-thermal simulator is necessary.

Thermal analysis of MEMS is usually done using finite element (FE) simulation. However, when electronic subsystems appear as dynamic heat sources, one needs system-level simulation with transient thermal fields included, which is outside the scope of standard FE simulators.

Therefore, dynamic thermal coupling between electronic subsystems requires a circuit simulator. In order to provide the capabilities of transient electro-thermal simulation, several forms of modelling have been proposed.

A widely used approach for coupled electro-thermal simulation exploits electronic equivalents of thermal networks using the finite difference method (FDM) for discretization. However, the FDM shows significant deficiencies when applied to irregular regions [4]. The finite element method (FEM) may also be implemented as an equivalent circuit network [5]. This approach is applicable for 2D simulation but in the case of 3D problems the number of passive elements grows beyond acceptable limits. In the MEMS field there is an increasing demand for reliable thermal simulation systems such as described in Ref. [6]. Simulators of this kind are based on the Fourier transform method which, however, is restricted to rectangular shapes. In addition, there are methods based on calculations of thermal impedance of arbitrary shaped heat generating regions using the thermal impedance of the sphere [7]. This could be used for fast electro-thermal estimations in non-layered and homogeneous structures. Other types of electro-thermal simulators are based on mixed-mode device simulators [8,9] with built-in compact models for analogue electronics. Such tools are capable of simulating accurate subsystem-level models consisting of several devices, including space-continuous thermal effects and analogue electronics. They are not intended for the system-level modelling consisting of complex analogue/digital networks with optional physical domains defined at various levels of abstraction (see Fig. 8).

Our objective is to provide a method for the simulation and verification of complete smart systems. This paper proposes the application of an event-driven mixed-signal simulator with an analogue hardware description language (HDL) for the system-level simulation of transient electro-thermal problems, without the need to derive any electronic equivalents of thermal networks. By using a mixed analogue/digital simulator environment and a FE description of the thermal problem coupled with electronics, one may effectively simulate analogue/digital electronics and thermal fields. Hence, the modelling is significantly simplified and the models may be imported directly from commercial FE simulators. Furthermore, this principle is flexible enough to be used in the analysis of other coupled field problems. Therefore, a 'universal' system-level analysis tool might be derived from an analogue simulator environment.

2. Description of the approach

The user defines the geometry and position of the components on the wafer using commercial FE software with meshing capabilities. The equation system is extracted and brought into a form applicable to analogue simulators. Afterwards, the electronic system, or components described on higher level of abstraction are defined and coupled with thermal FE modules.

The ALECSIS simulator [10] equipped with the ALEC++ analogue HDL is used for simulation (see Fig. 1). The architecture of this simulator is similar to other commercial analogue simulators [11,12], but extends the capabilities for the description of space-continuous models in an object-oriented HDL. This permits the calculation of the entire system in a single system matrix, thereby avoiding the use of relaxation methods. According to the work of Senturia [13], the relaxation procedures are not particularly reliable for the simulation of closely coupled physical domains in heterogeneous simulation environments.

Due to increasing computational expense, it is not suitable to treat each transistor on the chip as an individual heat source. Instead, regions with small power dissipation are neglected and highly dissipative circuit areas are represented by a suitable distribution of heat sources. This requires lower mesh densities in thermally 'inactive' regions, enabling a faster simulation. Such an approach is particularly meaningful for transient calculations.

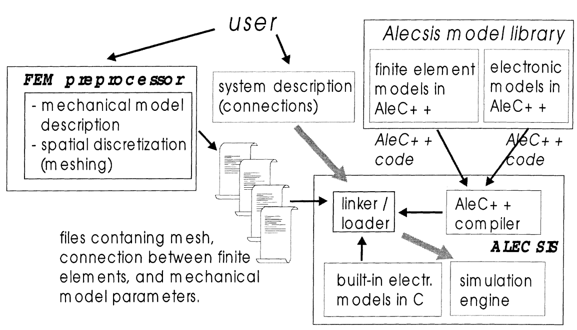

Fig. 1. Description of the simulation approach.

The strength of the method is in fact that FE discretization can accurately describe the physical laws on irregular shapes with unstructured mesh. Therefore, better accuracy is achieved for an equal number of nodes, in comparison with FDM calculated with structured mesh.

3. Theoretical background of the method

Transient thermal problems are analyzed by solving the heat transfer equation:

$$k\Delta T - \rho \times c\frac{\partial T}{\partial t} + q^{\mathrm{V}} = 0 \tag{1}$$

where T is the temperature and k, c, ρ and q^{V} denote the thermal conductivity, heat capacity, material density and the volumetric heat flow, respectively.

In most cases the boundary conditions are such that either temperature or heat flux are prescribed at the surface S of the body. Accordingly,

$$T = T^{\mathrm{S}} \text{ on } S_T, \quad q_n = k\frac{\partial T}{\partial n} = q^{\mathrm{S}} \text{ on } S_q, \tag{2}$$

where S_T and S_q, respectively, denote the surface with prescribed temperature or heat flux. In Eq. (2) $\partial T/\partial n$ is the directional derivative of the temperature field along the outward normal vector $\mathbf{n}$ on the boundary S. Eqs. (1) and (2) are the result of minimizing the functional [14]

$$\Pi = \int_V \frac{k}{2}\left[\left(\frac{\partial T}{\partial x}\right)^2 + \left(\frac{\partial T}{\partial y}\right)^2 + \left(\frac{\partial T}{\partial z}\right)^2\right] \mathrm{d}V - \int_V T(q^{\mathrm{V}} - \rho c\dot{T})\,\mathrm{d}V - \int_S Tq_n\,\mathrm{d}S \tag{3}$$

Within each finite element the temperature distribution is represented by the nodal values comprised in the vector $\mathbf{T}^{\mathrm{e}}$ and a suitable set of shape functions collected in a matrix $\mathbf{H}(\mathbf{x})$, such that

$$\mathbf{T}(\mathbf{x}) = \mathbf{H}(\mathbf{x})\mathbf{T}^{\mathrm{e}} \tag{4}$$

The temperature gradient grad T can be written as

$$\operatorname{grad} T = \mathbf{B}\mathbf{T}^{e} \tag{5}$$

with

$$\mathbf{B} = \begin{pmatrix} \partial\mathbf{H}/\partial x \\ \partial\mathbf{H}/\partial y \\ \partial\mathbf{H}/\partial z \end{pmatrix} \tag{6}$$

Introducing this into Eq. (3) and performing the extremum principle $\delta\Pi = 0$ for a single element yields the following equations for the nodal temperatures (see, for example, Ref. [14] for further details):

$$\mathbf{C}\dot{\mathbf{T}}^{\mathrm{e}} + \mathbf{K}^{\mathrm{V}}\mathbf{T}^{\mathrm{e}} = \mathbf{Q}^{\mathrm{V}} + \mathbf{Q}^{\mathrm{S}} \tag{7}$$

with

$$\mathbf{K}^{\mathrm{V}} = \int_{V^{\mathrm{e}}} \mathbf{B}^{\mathrm{T}}k\mathbf{B}\,\mathrm{d}V, \quad \mathbf{C} = \int_{V^{\mathrm{e}}} c\mathbf{H}^{\mathrm{T}}\mathbf{H}\,\mathrm{d}V, \tag{8a}$$

$$\mathbf{Q}^{\mathrm{V}} = \int_{V^{\mathrm{e}}} \mathbf{H}^{\mathrm{T}}q^{\mathrm{V}}\,\mathrm{d}V, \quad \mathbf{Q}^{\mathrm{S}} = \int_{S_q} \mathbf{H}^{\mathrm{T}}q^{\mathrm{S}}\,\mathrm{d}S. \tag{8b}$$

A global description of the system is obtained by assembling the system of equations for each finite element. The resulting system of ordinary differential equations is solved by analogue simulator. The entire system-level model is assembled from finite elements and compact electronic device models programmed as libraries in ALEC++.

4. Description of results

At first the method is tested on simply shaped structures, which are analyzed by an analogue simulator and compared to the results of an FE computation using ANSYS v5.4. An example of such 2D structure (ANSYS simulation) is shown in Fig. 2. Similar structures may be found in IC design problems, where heat dissipating (power) devices as well as other digital and analogue components are located on the same wafer. Fig. 3 represents simulation results for the same problem, using ALECSIS. Thereby the parameters for the calculation of the matrices $\mathbf{K}^{\mathrm{V}}$, $\mathbf{C}$, etc., are extracted from the ANSYS output data and solved in ALECSIS. The maximal relative error between the two simulators over arbitrary two-dimensional models with triangle-shaped finite elements is less than 0.005%. This, for the moment, merely demonstrates the correct transfer of thermal model from ANSYS to the analogue simulation environment. As explained in Section 2, only those components that dissipate considerable energy are modelled as heat sources.

The quality of this approach becomes obvious in problems consisting of MEMS structures with irregular shapes. One example is a class of flow sensors based on the anemometry principle. Those are widely used in miniaturized devices [15,17,18]. The heater is employed for generating thermal gradients in the region of interest (wire, cantilever, bridge). The temperature difference between the referent and the heated position is proportional to the velocity of flow, since the flow disturbs the distribution of thermal gradients. Such a system is shown in Fig. 4 and its principle of operation is similar to the system described in Refs. [15,16]. It is also possible to construct a system capable of

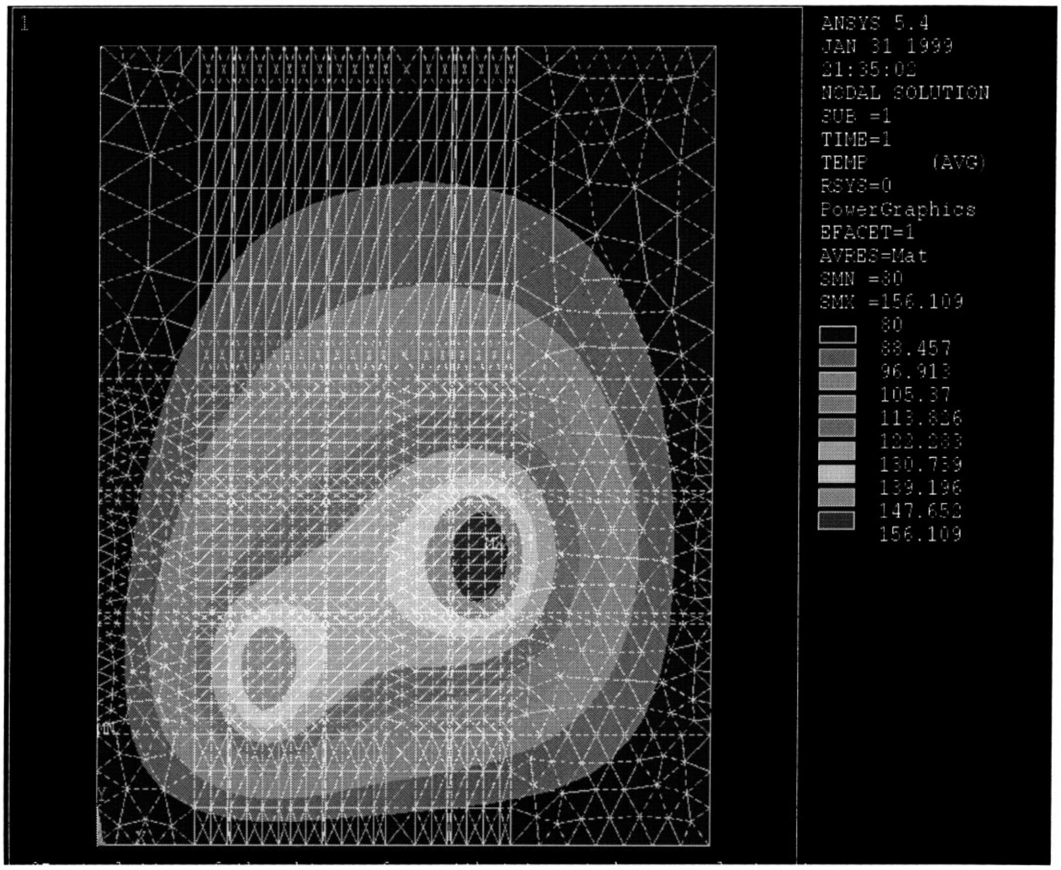

Fig. 2. Temperature distribution on the chip with two heat-dissipating regions (calculated by ANSYS v5.4).

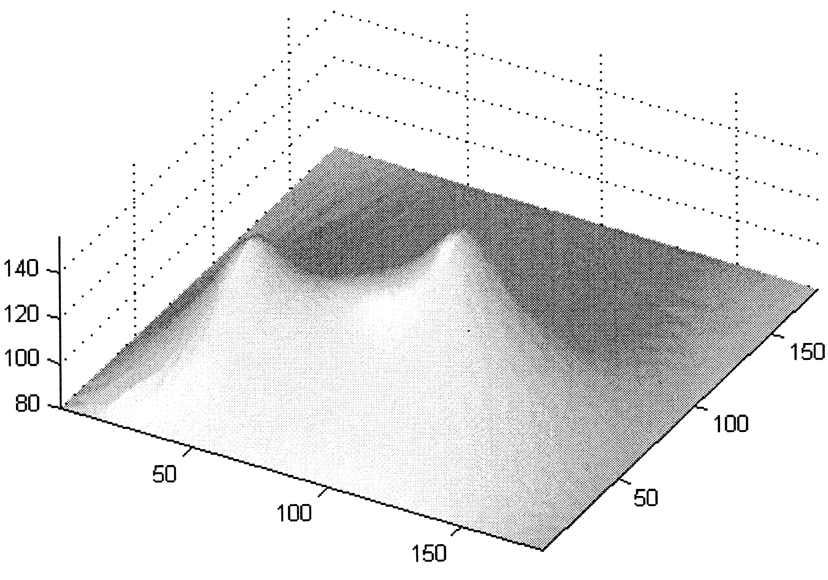

Fig. 3. Temperature distribution on the chip with two heat-dissipating regions (ALECSIS simulation/MATHCAD visualisation).

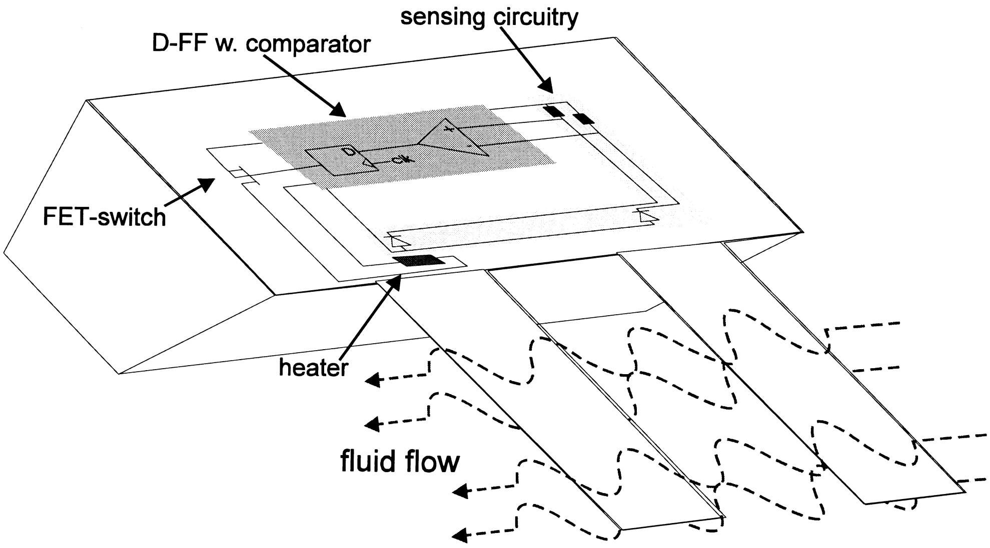

Fig. 4. The flow sensor with the circuitry.

measuring bi-directional flows. This requires also the second reference on the opposite side of the first one, positioned symmetrically with respect to the heater.

The device [15] takes into account the forced convection caused by the fluid. This kind of heat dissipation will be emphasized, if the speed of the fluid increases. This in turn causes an increased heat transfer to the fluid. A pulsed heat source should be activated more frequently, in order to preserve the constant temperature difference between cantilevers.

The coupled simulation of such systems cannot be realistically evaluated in any simulator environment other than the analogue simulator with HDL. It is a fluidic-thermal-electric system and requires simultaneous treatment of all participating physical domains. The assembly of the sensor components is shown in Fig. 4. The circuit maintains a constant average temperature difference between the heater and the reference. The thermal flow is governed by the fluid flow and is measured by the temperature-dependent diodes (S_{H} and S_{REF}), Fig. 5. Similarly, the heater is a non-linear temperature dependant component.

This system represents a sigma-delta converter of the first order with a low-pass feedback incorporated in the thermal system (Fig. 5). The FET transistor is switched depending on the temperature difference between the heater and the reference, in order to maintain the predefined difference. The frequency of the switching is the measure of the flow velocity.

4.1. Model description

The ANSYS simulator is employed as a pre-processor. The ANSYS results are also used for verification of thermal models in comparison to steady-state FE simulations by the analogue simulator. These models may be automatically converted into the ALEC++ format.

The problem is split into a compact (analogue and digital) and a space-continuous (thermal) part. Lumped models of electronic components have the same temperature as one of the inputs. Component RH emits the heat into a predefined volume of constant density, Fig. 5. The non-linearity of diodes and heater are fully taken into account.

If necessary, electronic components can be represented as distributed, instead of compact (lumped) models. In this case an electronic component will be composed of several finite elements.

The interaction between fluid and cantilever is

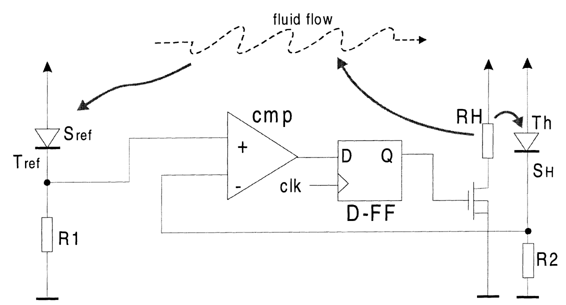

Fig. 5. Electro-thermal sigma-delta converter [19] with thermal flows in the system.

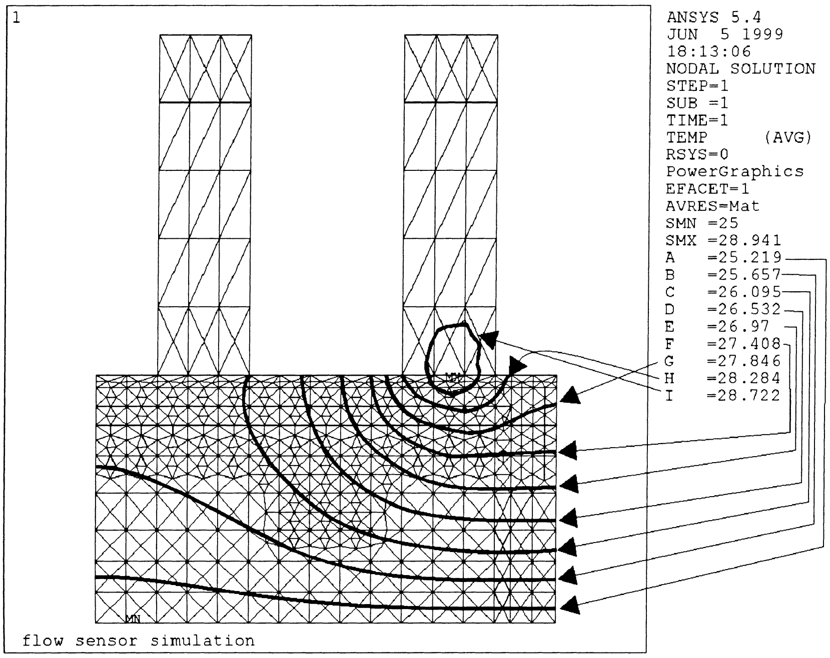

Fig. 6. Temperature distribution on the chip.

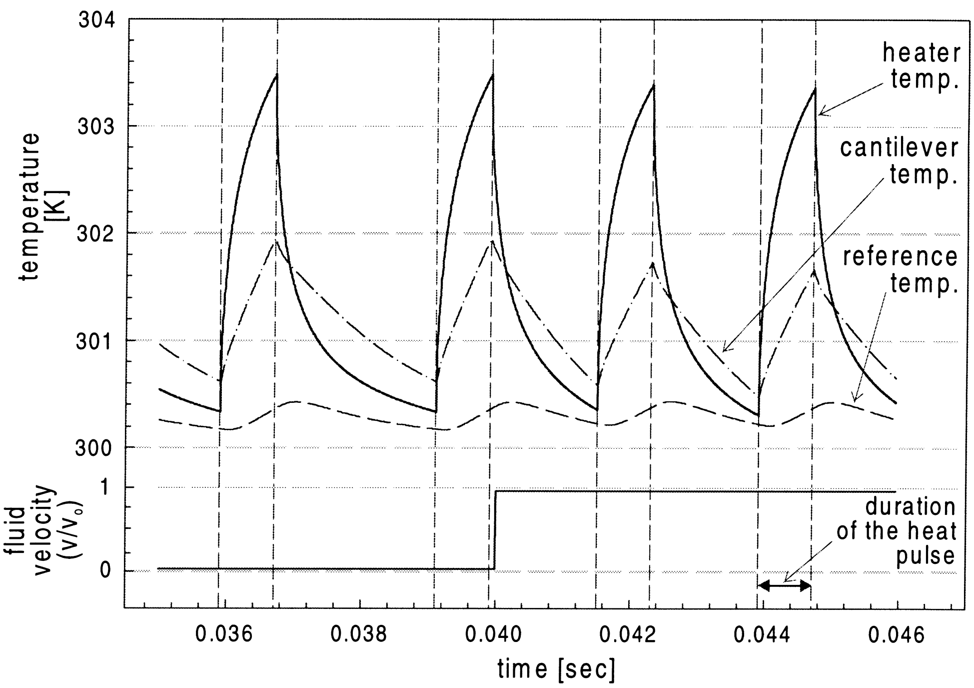

Fig. 7. Transient results for the behaviour of the 3D flow sensor (ALECSIS simulator). The traced signals are the fluid velocity, the temperature of the heater, of the cantilever close to the heater and the temperature of the reference diode.

modelled as forced convection [15]. This model is organized as an array of behavioural models and each of them is connected to the particular finite element of the cantilever.

4.2. Performances and benchmarking

The ANSYS v5.4 results for a 2D thermal simulation with emphasized isotherms are shown in Fig. 6. Comparison with ALECSIS results shows a relative error $< 0.002\%$ [22]. The 2D model has been somewhat simplified. The bottom part of the structure in Fig. 6 is exposed to a fixed temperature, presuming the connection to an ideal sink. Additionally, the system is taken to be adiabatic in the z-plane, i.e. there is no heat transport in the direction of the z-axis. The electronic

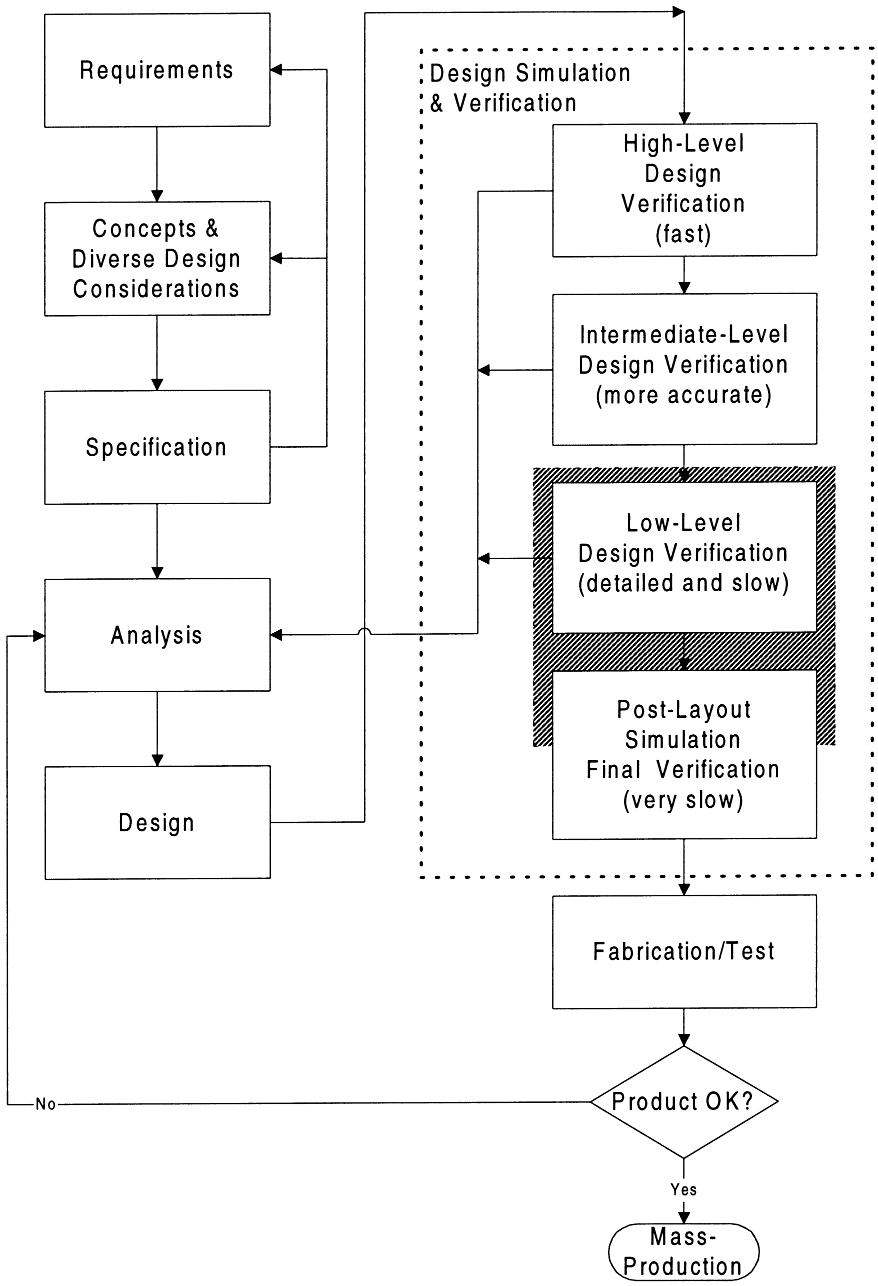

Fig. 8. The field of application for proposed electro-thermal simulation method (shaded region).

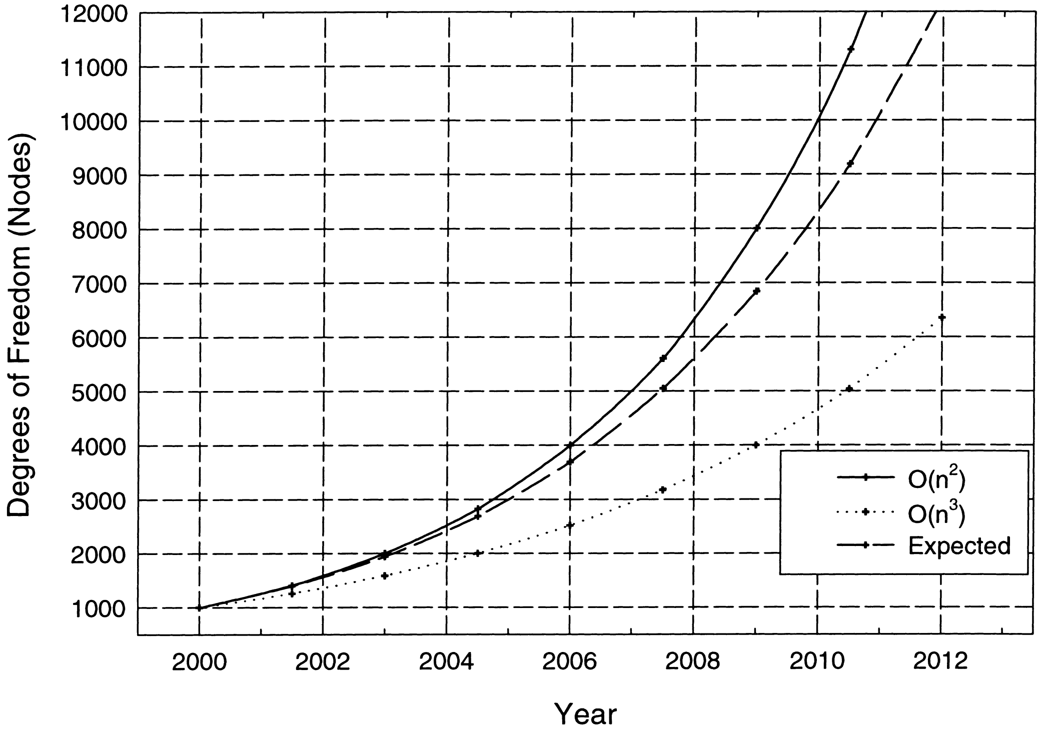

Fig. 9. Future outlook for the simulation of complex electro-thermal systems (simulation time ~45 min).

components are infinite in the z-plane, which is a very rough simplification even for a very thin wafer. This simplified model serves as a starting point for examination of the modelling capabilities of analogue simulators.

Transient simulation results of the coupled electro-thermal system are shown in Fig. 7. Traced signals represent the temperature of the heater and the cantilever close to the heater as well as the reference temperature and the fluid velocity. Note the change in the heat pulse frequency as a result of the change in fluid velocity.

We have performed a number of tests to evaluate the accuracy and speed of our approach. Three-dimensional simulations using tetrahedral elements have been performed and the results agree to within 0.08% for steady-state computation in comparison to ANSYS. For a typical transient simulation consisting of the thermal model with 1159 nodes and coupled electronics, calculated in approximately 30,000 time and iterative steps the computation takes approximately 4 h on an up-to-date workstation. The number of required time steps and non-linear components could significantly influence the simulation time. For static calculations with plain thermal models and 30,000 nodes a computation time of approximately 15 h is needed using a frontal solver. With the current capabilities of direct solvers in analogue simulators, transient simulations of 3D models with < 10,000 nodes can be accomplished within acceptable time spans.

In other words, the critical operating conditions of a fully coupled transient electro-thermal model can be simulated in 5–7 days. According to the location of this method in the hierarchical design flow (Fig. 8), it might be an option for accurate electro-thermal modelling at the end of the verification cycle and prior to the fabrication of mixed/analogue systems and microsystems.

4.3. Future outlook and performance estimate

Depending on the simulation task, the number of degrees of freedom (DoF) is between $N \times 1000$ and $N \times 10^6$ (with $1 < N < 10$). Two-dimensional problems require around 10^3–$N \times 10^4$ DoF, while the 3D thermal simulations require at least $N \times 10^3$ nodes. Direct sparse solution methods solve systems of equations of order n with $O(n^2)$ [21], rather than $O(n^3)$ multiplications, since the factorization is performed only once. This means that with the present computing resources in analogue simulators the calculation of highly complex problems cannot be accomplished within a reasonable time. However, the speed of computers doubles every 18 months [20]. With this tendency, our approach will be applicable to problems of higher complexity in the near future.

Since space-continuous coupled simulation tasks require large computational efforts, they are performed as the finalt verification step, Fig. 8. However, we should consider future problem solving and so it seems meaningful to estimate the applications area of our approach with computers of tomorrow. Taking into account the above mentioned increase of the computation speed as well as the dependence of the simulation time on the number of nodes, we obtain the following relation:

$$\tfrac{1}{3}n^3 + TI \times n^2 = k \times 2^{Y-2000/1.5} \qquad (9)$$

where n denotes the number of nodes, TI is the number of iterative and time steps, Y is the calendar year and the k is a constant. This describes transient thermal models with 10^3 nodes simulated in 5000 steps taking approximately 45 min at the beginning of the year 2000. The future perspective on the complexity of electro-thermal problems is shown in Fig. 9. The y-axis shows how many DoF might be tackled in a particular calendar year with constant time consumption (45 min per simulation run). The intermediate line reveals the predicted performances. For more steps, the results will be closer to the $O(n^2)$ line (see Fig. 9).

This future outlook reveals the computation performances sufficient for transient simulations in a large spectrum of electro-thermal designs. We may conclude that the proposed method will be shifted towards intermediate levels (Fig. 8) of design verification. The complexity of transient electro-thermal models might exceed 10^5 DoF before the end of the next decade. Major breakthroughs should emerge from the field of iterative solver technology, capable of calculating similar problems with $O(n^2)$ for a huge number of DoFs ($\sim 10^6$), especially on parallel computer architectures. Under these aspects, this approach is expected to gain momentum in the years to come.

5. Conclusion

The capability of analogue simulators for transient electro-thermal analysis has been presented. The designer is permitted to model both electronic networks and thermal space-continuous systems simultaneously, without a need to idealize the thermal subsystem. This method may be particularly attractive in the field of microsystem/IC design and verification, where other methods for transient electro-thermal simulation have either insufficient accuracy or are not feasible at all. Furthermore, a link between different physical domains may be easily established [22].

The superb quality of discrete circuit models available in analogue simulators, coupled with accurate continuous thermal models, could stimulate new applications in the field of transient electro-thermal simulations. Particularly, the reliability of microsystems in dependence of varying operating conditions and their periodicity through the device lifetime could be determined.

Acknowledgements

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