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NON-LINEAR NON-ITERATIVE TRANSIENT INVERSE CONJUGATE HEAT TRANSFER METHOD APPLIED TO MICROELECTRONICS

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ABSTRACT

Solving for temperature profiles given boundary conditions, geometry, and material properties is relatively straightforward given the wealth of analytical and computational techniques available. However, experimentally we often measure temperatures and seek to understand unknown boundary conditions or material properties. This problem is generally ill-posed. Thus, to get the value of these input parameters, we use inverse methods: knowing the output of the system (*i.e.*, temperature), we can compute the value of the unknown parameters (*e.g.*, thermal conductivity or heat fluxes). In microelectronics, the location and magnitude of the boundary conditions including local heat generation rates are often unknown or difficult to model due to the compactness of the current microchips and active thermal management schemes that distribute computations between different cores causing time-varying heat generation within the chips. This information can be retrieved using inverse heat transfer methodologies by tracking the temperature distributions in space and time. In this work, we develop a new, non-iterative inverse methodology to retrieve the heat flux inside of 3D geometries of stacked microchips. This method not only provides good agreement between the imposed and the retrieved heat flux with a linear form of the heat diffusion equation, but also predicts the imposed heat flux with good accuracy in situations with non-linearities. Here we numerically and experimentally validate our new approach using a microchip with 25 heaters that can be operated independently to create different

spatial and temporal heat flux patterns. During testing, the system is in a controlled environmental chamber and the temporal and spatially varying temperature of the top surface of the chip is measured using infrared thermography for input to the inverse method. The system and model include non-linearities through varying convective heat transfer boundary conditions on different parts of a test article and temperature-dependent thermal properties of the constituent materials. The inverse methodology retrieves the local heat generation rates with good agreement in time, space, and magnitude. An uncertainty analysis of the computation and the experiments is also detailed. Our methodology is unique compared to past work because non-linearity is solved without the need of using iterative processes, which makes the algorithm computationally efficient. Ultimately, this method is useful for the determination of the location and magnitude of the heat flux in any 3D system based on external temperature measurements with real heat transfer properties without the need of an iterative procedure.

INTRODUCTION

While it is relatively simple to measure temperature (*e.g.*, with thermocouples, infrared cameras, or resistance temperature detectors (RTDs)), it is challenging to measure local heat fluxes, especially in operating devices. Therefore, it is not uncommon to use temperature measurements in order to compute heat flux through an interface. In general, in inverse heat transfer problems, an unknown parameter (*e.g.*, heat generation rate, material property) or boundary condition (*e.g.*, heat flux, convection coefficient) can be retrieved by observing the temperature results. In these problems, the input is the temperature distribution and the output is the unknown parameter(s). Such problems are ill-posed and the solution is not unique [1]. That is, different combinations of parameters (*e.g.*, different distributions of heat fluxes) will give similar temperature distributions and small variation in the input parameters can lead to large fluctuations in the solution.

Inverse methodologies can be divided in linear methodologies and non-linear methodologies, depending on their capability to solve non-linear problems. The linearity of the inverse problem is set by the temperature dependency of the boundary conditions and thermal properties of the materials. Methods based on Duhamel Theorem [2]-[5], and Laplace transforms [6][8] fail to solve non-linear cases since their solutions are based on linearizing the heat diffusion equation. For this reason, differential approaches [9][13] are used to solve non-linear inverse problems. As the temperature is needed to retrieve the thermal properties, a common thought is that the differential approaches need to be iterative to solve the non-linear problems, *e.g.*, the Levenberg-Marquardt method [14]-[16].

In this paper, we present a novel non-iterative non-linear methodology to solve inverse problems. In order to avoid iterating, the method leverages the fact that the surface temperature distribution, which would be part of the solution of the direct problem, is known and an input of the problem from the beginning. Therefore, we can estimate the thermal properties of the materials as a function of space and time immediately. With this simplification that can be done beforehand, the heat diffusion equation can be linearized even with temperature dependent thermal properties and boundary conditions. Combining this methodology with the Digital Filter Method [17] [18], the inverse solution can be obtained in seconds, and therefore, using proper solving algorithms, it can be solved in near real time.

This method is particularly useful for microelectronics as in every processor and many other components, there are embedded temperature sensors, but there are not heat flux sensors. Consequently, the temperature is the only information that we have about the thermal behavior of the microchip. Inverse methods can retrieve the local and instantaneous heat flux, and other parameters that are unknown. The application of this new method (solving almost real time inverse problems including non-linearities) could enable active control of the thermal behavior of different electronic devices. The location of temperature sensors can also be optimized in the design phase, based on the magnitude and proper determination of the location of the heat sources [19]. Due to all these benefits, we validate the non-iterative methodology using a microchip with twenty-five independent heaters. The temperature distributions on the graphite-coated top surface of the microchip are measured with an infrared microscope and imposed heat patterns are retrieved within seconds using the non-linear, non-iterative method. Evaluation of the uncertainty in the predictions shows that the method is primary sensitive to the temperature measurements, and the thermal properties of the materials are not negligible in the uncertainty assessment.

NON-LINEAR NON-ITERATIVE INVERSE CONJUGATE HEAT TRANSFER METHODOLOGY

We previously developed the digital filter method for linearized conduction problems (using COMSOL) and linearized conjugate heat transfer cases (using ANSYS Fluent) [19]. Here, we develop a new strategy to incorporate non-linear thermal properties and boundary conditions into the digital filter method.

The methodology consists of linearizing the heat diffusion equation to quantify the response of the system to the application of heat flux pulses through a sensitivity coefficient matrix. A sensitivity coefficient can be understood in layman terms as the quantification of the “effect” on a measured parameter due to a variation in a “cause”. Here, the sensitivity coefficient relate the temperature rise at a particular location and time (i.e., the “effect”) to variations in the input heat flux (i.e., the “cause”), which is similar to the concept of thermal resistances but evaluated at every

position and time within the domain. Mathematically it is expressed as the derivative of the temperature with respect to the heat flux at a particular location and for a 1D problem with a single heat source can be represented as:

$$X_{jM}(x_j, t_i) = \frac{\partial T(x_j, t_i)}{\partial q_M} \quad (1)$$

Therefore, X_{jM} represents the measured effect (temperature) at the location x_j at the time t_i due to the heat flux component q_M , where the subscript M represents the time step when the heat flux was applied. X_{jM} is the sensitivity coefficient that measures the sensitivity of the temperature measurement $T(x_j, t_i)$ to changes in the value of q_M . Small values of the sensitivity coefficient imply that large changes in the heat flux yield small changes in the temperature. The calculation and effect of the sensitivity coefficients have been studied previously for linear inverse problems [20].

These coefficients are computed by applying heat flux pulses at distinct locations in the test article and observing the spatially- and temporally-varying temperature increase. Therefore, a pre-assessment of the test article based on direct computations (*i.e.*, applying an arbitrary heat flux pulse and calculating temperature responses) generates the sensitivity coefficients prior to applying the inverse method, as described in Figure 1. In this case, in order to retrieve the sensitivity coefficient heat pulses of $1 \times 10^6 \text{ W/m}^2$ were applied in the central heater.

Figure 1. Schematic of the process to retrieve the imposed heat flux distribution using the Digital Filter Method (DFM). First, direct heat transfer computations are performed imposing heat flux pulses. Then, the predicted temperature with respect to the heat flux pulses are evaluated to generate the sensitivity coefficients matrix, X_{ij} . Combining these sensitivity coefficient matrix with the measured temperature map, $Y(x,t)$, enables extraction of the heat flux distribution, q_c .

The boundary conditions applied to get the sensitivity coefficients vary depending on the model: (1) a fixed convection coefficient ($h_{\text{conv}}=10\text{W/m}^2\text{K}$) is applied on all boundaries in the case of the conduction model and (2) appropriate conjugate boundary conditions based on modeling the fluid flow are applied in the case of the conjugate heat transfer model.

The sensitivity coefficient matrix is an array of coefficients distributed in time and space that represent the effect over the temperature in a particular point i at a particular time k , of a heat flux pulse in a location j . Therefore, the sensitivity coefficients are defined as follows:

$$X_{i,j}(k) = \frac{\Delta T_{i,k}}{q_{\text{pulse},j}}, \quad (2)$$

and are similar in concept to thermal resistances. Based on this notation, the construction of the sensitivity matrix takes into account the spatial discretization

$$X(j) = \begin{bmatrix} X_{11}(k) & X_{12}(k) & \cdots & X_{1p}(k) \\ X_{21}(k) & X_{22}(k) & \cdots & X_{2p}(k) \\ \vdots & \vdots & \ddots & \vdots \\ X_{m1}(k) & X_{m2}(k) & \cdots & X_{mp}(k) \end{bmatrix}, \quad (3a)$$

and it couples it with the temporal discretization

$$X_{\text{total}} = \begin{bmatrix} X(1) & 0 & 0 & \cdots & 0 \\ X(2) & X(1) & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ X(n) & X(n-1) & \cdots & \cdots & X(1) \end{bmatrix}, \quad (3b)$$

where m is the total number of sensors, p is the total number of heat sources, and n is the total number of timesteps.

The basic algorithm that describes this approach was introduced by Levenberg and Marquardt [16] for parameter and function estimation. This algorithm was initially developed to solve non-linear estimation problems, but it is used in this case to solve ill-conditioned linear problems. The estimation of the heat flux (or any parameter that we want to estimate using the inverse method) is based on the minimization of the ordinary least squares norm:

$$S(q_c) = \sum_{i=1}^M (Y_i - T_i(q_c))^2, \quad (4)$$

where S is the objective function, Y_i is the measured temperature, $T_i(q_c)$ is the estimated temperature, and M is the number of measurements. In order to minimize the above objective function, we need to compute the derivatives with respect to all the parameters we need to estimate and equate this to zero. The gradient of the objective equation with respect to the vector of heat flux needs to be equal to zero:

$$\nabla S(q_c) = -2 \underbrace{\left[\frac{\partial T^T(q_c)}{\partial q_c} \right]}_{X^T} [Y - T(q_c)] = 0. \quad (5)$$

The sensitivity matrix, X_{ij} , also known as Jacobian matrix, is the transpose of the first term between brackets in the equation 5, so that equation can be expressed using the sensitivity matrix as

$$-2 X^T [Y - T(q_c)] = 0 \quad (6)$$

If the sensitivity matrix of coefficients does not depend on the temperature, *i.e.*, we are solving a linear problem, the solution for the equation 6 can be expressed as

$$q_c = (X^T X)^{-1} X^T Y. \quad (7)$$

Equation 7 constitutes the main core of this method and provides the best estimator of the linear problem solution using least squares.

There have been two main expansions of this equation over the years in order to accommodate the solution for non-linear problems and to avoid the non-singularity of the matrix $X^T X$ due to the ill-condition nature of the problem. The non-linear estimation of the heat flux requires an iterative procedure. For this iterative process, the temperature vector is linearized using a Taylor series expansion around the solution of the heat flux at the previous iteration. The equation 8 linearizes the temperature behavior under non-linear conditions, where k is the current iteration.

$$T(q_c) = T(q_c^k) + X^k (q_c - q_c^k) \quad (8)$$

When we substitute the new value of $T(q_c)$ described in equation 8 into equation 6, the best estimator of the q_c is written as the iterative Gauss method which is an approximation of the Newton-Raphson method.

$$q_c^{k+1} = q_c^k + [(X^k)^T X^k]^{-1} (X^k)^T [Y - T(q_c^k)] \quad (9)$$

The solution proposed in the Digital Filter Method is a non-iterative solution that combines the Levenberg-Marquardt method with a regularization divided in a spatial term and a time term[17][18]. This regularization technique is used to avoid the issue of the sensitivity of the solution of the inverse methods to small variations. Therefore, the equation that needs to be fit is

$$S = (Y - T)^T (Y - T) + \alpha_t [H_t q]^T [H_t q] + \alpha_s [H_s q]^T [H_s q]. \quad (10)$$

The solution to this is obtained applying the same principles that in the Levenberg-Marquardt method:

$$q_c = [X^T X + \alpha_t H_t^T H_t + \alpha_s H_s^T H_s]^{-1} X^T Y. \quad (11)$$

Once the values of the sensitivity coefficients are obtained, we solve can solve system of equations where Y is the measured temperature. The regularization terms $\alpha_t H_t^T H_t$ (in time) and $\alpha_s H_s^T H_s$ (in space) help to solve the problem with an ill-conditioned sensitivity matrix by limiting the heat flux variations between adjacent time steps and heat source locations [21] [22] [23]. α_s and α_t are the regularization parameters with values between 10^{-12} and 0. The value of these regularization parameters vary depending on the spatial concentration of heat flux and the expected value for the second derivative in time of the variation of heat flux. When there are large spatial gradients the value of α_s is 10^{-12} while when small spatial gradients are expected the value is 0. Equally, when large temporal gradients are expected α_t is 10^{-12} and with flatter temporal distributions its value is 0. The procedure to select these values is detailed in [4]. The matrix H_s and H_t define the order of the regularization and they vary depending on the spatial arrangement of the heat sources and its location in the sensitivity matrix. For example, considering first order regularization terms in both space and in time these matrices take the following form:

$$H_t = \begin{bmatrix} -I & I & 0 & \dots & 0 \\ 0 & -I & I & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \dots & 0 \end{bmatrix}, \text{ where } I = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \dots & 1 \end{bmatrix} \quad (12 \text{ a, b, c, d})$$

$$H_s = \begin{bmatrix} h_s & 0 & 0 & \dots & 0 \\ 0 & h_s & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \dots & h_s \end{bmatrix}, \text{ where } h_s = \begin{bmatrix} -1 & 1 & 0 & \dots & 0 \\ 0 & -1 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \dots & 0 \end{bmatrix}.$$

Najafi *et al.* [18] used this method for simple 2D geometries.

Here, we improve the Digital Filter Method by modifying two terms in equation 3: (2) the adjusted sensitivity coefficient (X_T) by adding in the temperature-dependence and (2) the heat flux term (q_c) by including the convective heat losses (q_{conv}). Therefore, the heat fluxes are now defined by:

$$q_c = q_{imp} + q_{conv} = [X_T^T X_T + \alpha_t H_t^T H_t + \alpha_s H_s^T H_s]^{-1} X_T^T Y. \quad (13)$$

We focus on solving for the imposed heat flux, q_{imp} as the unknown in this inverse methodology with the temperature of the surface an input of the method. Hence, the convective heat flux can be computed beforehand from the difference between the flow temperature and the solid temperature at each discretize location:

$$q_{conv} = C (Y_i - T_{amb}). \quad (14)$$

The mathematical description of this formula is analogue to the mathematical description of the convective heat flux leaving the surface of the test article. More complex boundary conditions can be added depending on the expected importance of the different heat transfer modes. In this way we are linearizing the non-linearity that can be observed in the boundary conditions.

The coefficient C is a combination of the convective heat coefficient and the area where the temperature reading is averaged. This coefficient varies depending on the flow conditions, surface radiation and the studied geometry, therefore it needs to be calibrated before performing direct calculations at different conditions. For the studied cases, radiation was found negligible due to the small variations of temperatures experienced by the sample and the low emissivity value of the materials at ambient temperature [24]. Therefore, for this particular case, the coefficient C is primarily dependent on the convective heat transfer coefficient. Direct calculations with the natural convection and conjugate heat transfer models were performed in order to compute the coefficient C value, increasing from 150 W/m²K to 3000 W/m²K from the natural convection case to the conjugate forced convection case. Once the value of the coefficient C is obtained, the subtraction of the convective heat flux from the computed heat flux, q_c , will give the imposed heat flux.

Figure 2. Non-linear non-iterative process for estimation of the corrected sensitivity coefficient. Direct heat transfer computations(a) are performed at different test article temperatures to retrieve the relation between the sensitivity coefficient and the temperature response of the system (b). Knowing this relation, the temperature corrected sensitivity coefficient can be obtained.

The second improvement is the development of a new non-iterative methodology to include the non-linearity of temperature varying thermal properties in the inverse methodology. In order to mathematically explain the non-linearity carried out by the thermal properties, we recall the definition of the sensitivity coefficient from Equation 1. If we apply this definition to the Fourier's law for heat conduction in a 1D system, for simplicity, we obtain:

$$\dot{q}_c = -k(T) \frac{\partial T}{\partial x} \quad \rightarrow \quad q_c = -k(T) \frac{T - T_0}{L} \quad (15)$$

If we compute the sensitivity coefficient of the temperature with respect to the heat flux, we obtain:

$$X = \frac{T - T_0}{q_c L / k(T)} = \frac{k(T) \partial T}{L \partial q_c} \quad (16)$$

As can be seen, the conductivity $k(T)$ is dependent on the temperature of the material and introduces a non-linearity in the solution of the equation. This is the mathematical explanation for a simple case, but it can be extrapolated to more complex 3D cases where the heat conduction equation is solved with the non-linearity provided by the conductivity, but also of the density and the specific heat capacity.

Most methods that include this non-linear behavior, such as the Levenberg-Marquardt Method [16], are based on iterative processes that take into account the temperature obtained in the previous iteration in order to compute the new values of thermal properties. In the present study, the temperature is considered a known parameter since it is measured at each timestep, and considering the small thicknesses of the silicon layers, we neglect the variation through the sample thickness. The temperature varying thermal properties are modelled in the system using temperature varying functions and based on empirical data for the considered materials. The sensitivity coefficient can be adjusted based on the measured temperature before the inverse calculation is performed. The temperature adjustment of the sensitivity coefficients is made by running direct simulations with heat flux pulses at different temperatures of the test article. These simulations quantify how the temperature field reacts when the test article is at higher temperatures and, therefore, has different thermal properties. Figure 2 represents the process followed to obtain the temperature-adjusted sensitivity coefficients.

Note that the sensitivity coefficient changes when the temperature is increased (Fig. 2(a)) and the results of the heat flux pulse simulations at several temperatures are compiled (Fig. 2(b)). A linear fitting with respect to the test article temperature between the coefficients leads to the concept of temperature factor, F_T . The corrected sensitivity

coefficient is then obtained by multiplying of the temperature factor by the sensitivity coefficient at ambient temperature:

$$X_T = F_T X_{amb}. \quad (17)$$

With the temperature field at each timestep, the temperature factor F_T is computed using a linear fitting based on the data obtained with the heat flux pulses at different temperatures. Then the corrected sensitivity matrix X_T is obtained for each timestep. With this non-iterative method, the non-linearity due to the temperature varying thermal properties is introduced in the calculation. This improved methodology is used for the calculation of the heat flux in a microchip with 25 heaters independently controlled by measuring the temperature on the top surface with an infrared microscope.

NUMERICAL AND EXPERIMENTAL VALIDATION

Figure 3 shows the complete procedure for the validation of the inverse heat transfer methodology. As specified in the previous section, we need to compute the sensitivity coefficients in a first step. This is achieved numerically solving the heat conduction equation through COMSOL or ANSYS Fluent, depending if we solve the convective case or the conjugate heat transfer case.

Then numerical and experimental validations are performed where the inverse methodology is run using as inputs the temperatures maps obtained from the solution of the heat conduction equation and the measured temperature during the experiment respectively. It is worth to remark that the inverse methodology is not used in a direct mode to retrieve the temperature maps. Therefore, the numerical direct solution obtained solving the heat conduction equation and the inverse heat transfer solution obtained solving the linearized heat conduction approach with regularization technique, are different models, and hence we would not commit the inverse crime [25]. Similarly in the experimental validation, the direct model was not used.

Figure 3. Complete procedure followed to numerically and experimentally validate the inverse heat transfer methodology. It specifies the different models and equations used in the computation of each step. As it can be observed, the inverse model is only used to compute the imposed heat flux, while the direct model, solving the heat conduction equation provides the temperature map used as input for the inverse heat transfer model.

The equations that need to be solved for the direct model and the inverse model are specified in the Appendix. Also the boundary conditions that have been used for the different cases in the computation of the sensitivity coefficients and the numerical validation are specified in the Appendix and complemented in Figure 5.

First, we validate the methodology with numerical models that simulate the real environment and experimental setup. Then, several experiments with the test chip prove the viability of this inverse methodology for real applications. The experiments were performed using a 21x21mm microchip with 25 heaters and 26 embedded temperature sensors. Figure 4 shows the chip used during the experimental validation and a sketch of the location of the heaters inside the silicon layers.

Figure 4. Microchip with 25 independent heaters used for the experimental validation of the inverse methodology. The system consists of a grid with 25 independently controlled heaters and 26 embedded temperature sensors, with at least one temperature sensor within each heater cell.

Figure 5 shows two different models used for analysis of the microchip: (1) a pure conductive model using COMSOL Multiphysics® software and (2) a conjugate (*i.e.*, including convection and conduction) heat transfer model using ANSYS Fluent®. The COMSOL conduction model include the silicon microchip with several layers of silicon and 25 heaters embedded. The top surface is divided in a matrix of 25x25 pixels where the temperature is measured. The ANSYS Fluent conjugate heat transfer model includes several solid domains simulating the microchip, the printed circuit board (PCB), and a fluid domain simulating the air in the enclosure surrounding the chip. The fluid domain is modeled with a velocity inlet and a pressure outlet and the walls are slip walls, to avoid the generation of viscous heating in surrounding walls. The interface between fluid and solid domains is modeled as conjugate so we allow transfer of heat transfer between solid and fluid without imposing it. The thermal and geometrical properties of each layer are the same in both the pure conduction and conjugate model, and replicate the properties of the experimental test article. The temperature-dependent thermal properties, responsible for part of the non-linearity of the problem, are embedded within the ANSYS and COMSOL models. The heat flux boundary conditions are imposed using a boundary condition between solids, in the case of the COMSOL model, and a heat generation boundary condition within the Fluent model. This boundary condition generates heat at the interfaces between solids where the heaters are located. The conductivities and the specific heat capacities of the different materials, which determines the storage of heat within the system, are modelled based on the different materials that constituted the real microchip. In the appendix, the temperature dependence due to conductivity temperature variations in the silicon layer is detailed.

Figure 5. a) Microchip in the experimental setup including the enclosure used for temperature control, b) COMSOL model of the microchip with subdivisions in the top surface marking the approximate size of the pixels for IR thermal measurements, and c) ANSYS Fluent model of the microchip for conjugate heat transfer analysis with the flow boundary conditions. Divisions shown here outline the 25 different heaters elements.

To demonstrate the accuracy and feasibility of this inverse methodology, we first conduct a numerical “experiment” using the conjugate heat transfer model ANSYS Fluent. In this numerical experiment, first we compute the direct problem with known boundary conditions (*i.e.*, applied heat fluxes) in the heaters and measure the predicted temperature on the top surface of the silicon layer. In the inverse problem, we input the temperature measurement from the direct problem to compute the heat flux boundary conditions in space and time. In this way, we can compare the input heat flux boundary conditions to those delivered by the inverse method to assess the accuracy of the inverse approach. The objective of this test is to validate if the inverse methodology can predict the amplitude of the heat flux, the temporal evolution of the heat flux, and the spatial location of the heat source.

When a simplified inverse model is applied in order to solve the heat transfer problem, we can incur in the “inverse crime” if the discretization of the inverse model is coarser than the discretization of the direct model used to develop the method [25]. The simplified model used to retrieve the heat flux has been used for decades and validated through the years with analytical and finite elements solutions [4][6][9][11][15][16][17][21]. In order to avoid the “inverse crime”, the discretization in the direct solution is the same as that in the inverse problem solution. Additionally, the

prevention of the inverse crime is verified with the experimental validation and the application of Monte Carlo simulations with the same algorithm for gas turbine applications [26].

Specifically, in the numerical experiment, a single heater provides a sinusoidal heat flux over 10 seconds with a maximum amplitude of $2 \times 10^5 \text{ W/m}^2$. This is treated in the numerical model as heat generation from the heater surface. The remaining heaters are off for the entire duration. In the simulations, the rest of the boundaries were set as for the calculation of the sensitivity coefficients. Additionally, the velocity of the flow in the domain was input as 3m/s at the inlet of the domain.

Figure 6 depicts the imposed heat flux in four different heaters and the estimation of heat flux using the developed inverse methodology. Note that three heaters with no applied heat flux are shown for illustration and all the imposed and retrieved data for those heaters overlap at the 0 W/m^2 axis. The method accurately predicts the location of the heat source, the time evolution of the imposed heating, and the magnitude of the heat flux with an error below 5% of its maximum, only providing the temperature measurement of the top surface of the test article.

Figure 6. Numerical validation of the inverse methodology in ANSYS Fluent including conjugate heat transfer. (a) The imposed and retrieved heat fluxes as a function of time. (b) Top view of the 5x5 heater grid with the four selected heaters labeled. A heat flux is imposed on heater 1, while all remaining heaters are off for the duration of the simulations. Note that in (a) all data (imposed and retrieved) for heaters 2, 3, and 4 that were not “on” overlap at 0 W/m^2 . The data for heater 1 matches well in the amplitude of the peak heat flux with a slight delay during the offset in time where the heat flux is decreasing.

Subsequently, the methodology was evaluated experimentally using the microchip with 25 heaters (depicted in Figure 5a) in a controlled environment. The temperature-controlled enclosure was designed to contain the chip during

the calibration of the IR microscope in order ensure approximately uniform temperatures in the enclosure and during the experiments to better control the convective boundary conditions to which the chip is exposed. This enclosure is made with an aluminum structure and acrylic walls. In two parallel walls, two fans can blow air into the enclosure to supply forced convection heat transfer to the system. The temperature of the box is monitored in three different locations with thermocouple probes inserted through orifices in the different walls.

An infrared microscope (Quantum Focus Instruments Infrascopes) measures the temperature at the top surface of the microchip as a function of space and time with $\sim 18 \mu\text{m}$ spatial resolution and $\sim 0.1 \text{ K}$ temperature resolution. Because silicon is IR transparent, we apply a thin layer of graphite paint on the measured surface. The emissivity value measured by the infrared microscope during the calibration is 0.9 and it is uniform in all the field of view. The lens used in this experiment had a field of view of $12\text{mm} \times 12\text{mm}$, therefore, the experimental campaign was carried out using a 3×3 heaters array located in one of the corners of the test article, as shown in the Figure 7.

Figure 7. (a) Experimental setup to measure the top surface temperature of the chip in the specified field of view of the IR microscope. (b) Close up of the enclosure used for controlling convection and environmental temperature during calibration of the emissivity. (c) Schematic of the heater grid on the microchip indicating the field of view of the microscope.

The calibration of the setup was completed following three steps: (1) thermocouple calibration, (2) RTD and heater calibration, and (3) IR microscope calibration. The first two calibration steps were performed out of the experimental setup but using the same data acquisition system as during the experimental campaign. Three thermocouple probes were manufactured and calibrated using a temperature sensor dry bath calibrator able to keep the uncertainty of the bath below $\pm 0.003\text{K}$. The calibrated thermocouples were used to track the internal temperature of the oven where the Resistance Temperature Detectors (RTDs) and the heaters were calibrated at temperatures ranging from 308K to 363K. Figure 8 shows the behavior of the resistance with respect to the temperature of eight RTDs and the nine heaters used in the experimental campaign. Heaters and RTDs increase linearly their electrical resistance with the temperature, in the temperature range of interest. These calibrations are taken into account when computing the internal temperature of the microchip and the input power to the individual heaters. The RTDs are used to calibrate the IR microscope, as a safety check to monitor the temperature of the chip during the experiments, and to control the input heat flux so as not to damage the microchip.

Figure 8. a) Calibration of the RTDs that monitor the internal temperatures of the chip and b) calibration of the heaters located within the field of view of the microscope. Note that in both cases, the resistance increases linearly with temperature.

Prior to the thermal experiments, the IR microscope is calibrated with the final experimental setup in place. The sample is heated to a uniform temperature of around 323K. We then take a radiance image of the top surface and the knowing the temperature of the chip, the spatially-varying emissivity of the surface computed. This emissivity map is assumed to be constant for the relatively small range of studied temperatures and is used to obtain the temperature distributions of the measured surface.

In the experimental campaign, we performed different experiments with six different spatial distributions of heat flux under two convection cases: (i) natural convection with stagnant air in the enclosure and (ii) forced convection by using the fans installed in one of the sides of the acrylic box. Each experiment was run for 100 seconds recording one temperature map each second. In terms of time distribution of heat flux, the selected heaters for each of the cases were turned on between 2 s and 8 s after beginning the recording and they were switched off after 60 seconds of operation at constant heat flux. The heat flux generated by the heaters is controlled with a Labview program coupled with a Keithley sourcemeter, which is also used to record and save the data. The input Joule heat flux to each heater is calculated from the power supplied to the system, monitoring electricity voltage and current into each heater circuit. Figure 9 depicts the six experiments with variations in the heat flux maps and resultant temperature profiles. In this work we focus on experiments 1, 3, and 4 to validate the proposed inverse methodology.

Figure 9. Experiments performed to validate the methodology. Each small inset indicates which heat sources were on (orange) for each experiment and the black box indicates the field of view of the infrared microscope. The thermal images are from one frame of the thermal movie and show the spatial variation in temperature of the die.

As observed in the Figure 9, the spatial distribution of temperature varies considerably amongst the different experimental cases, this helps in the determination of the location of the heat sources and the retrieval of the value of the applied heat flux. In experiment 1, we powered the 3x3 grid of heaters within the field of view of the microscope, while in experiments 2 and 4 we only powered one heater but in different locations of our temperature map. In experiment 3, we used 2 heaters at the corners of the field of view. In the experiment 5 and 6, we turned on three heaters corresponding to a column and a row of heaters of the field of view, respectively. The temperature map obtained

with the IR microscope contains 1024x1024 measurements (pixels). To apply the inverse methodology, in which number of operations is directly proportional to the number of temperature measurements, we decided to reduce this number of measurements to a grid of 15x15 effective pixels. The temperature map was divided in the desired grid and all the nodes contained in the subdivisions were averaged at each time step to get the input temperature maps for the code. All the tested experiments were analyzed using the inverse methodology, but for the sake of conciseness in this paper we will focus on three of them: experiment 1 which is the most general case, and experiment 3 and 4 since they are the most challenging heat distributions of the experiments.

Figure 10. a) Experiment 1 where the whole field of view is heated and the temperature field is measured using an IR microscope. b) Imposed and retrieved heat flux using the Digital Filter Method algorithm without correcting for non-linearities.

First, consider experiment 1 where all the heaters in the field of view are operating at the same heating rate. In order to evaluate the importance of the non-linearity in this particular validation case, the inverse algorithm was first applied without correcting for non-linearities. As evident in Figure 10, the inverse method can retrieve the sudden changes in heat flux, but the magnitude of the heat flux is completely incorrect, which gives an indication of the importance of non-linearity in the problem.

When the inverse method is applied with the non-linear correction (see Figure 11), a considerable improvement in the accuracy of the prediction is rendered obvious. The temperature evolution in time is represented in the Figure 11 and we observe that we can predict the evolution in time of all the heaters. Also, the magnitude of the heat flux is captured well by the inverse methodology. The results show good agreement for both natural convection and conjugate heat transfer calculations.

Figure 11. Validation of the inverse methodology for the experiment 1. (a) Temperature maps at selected times. Note that the temperature is fairly uniform at each time step. (b) Sketch of the 5x5 heater grid with the 9 active heaters indicated in Figure 9. The black outline indicates the field of view. (c - d) Heat flux in the center (blue) and (red) corner heater within the field of view as extracted from the inverse method. Panel (c) shows the results for natural convection with the COMSOL model and panel (d) shows the results under forced convection using the ANSYS Fluent model.

The new methodology can predict, not only the magnitude of the heat flux and the temporal behavior of the heat flux, but also spatially resolve the locations of applied heat flux as shown in Figure 12 which illustrates the imposed and retrieved heat flux at $t=40s$ for experiments 3 and 4. We applied our methodology to the most complex case (experiment 3 where two heaters are active, while the rest do not provide any heat) and we obtained very good agreement in terms of the predicted magnitude of heat flux, the time when the heaters are turned on and turned off, and the location of the heat sources as can be observed in the Figure 12. The magnitude of the heat flux also varies from test to test and the methodology was able to compute the value of heat flux that was imposed with a reasonable accuracy ($< 10\%$ error) in all the heaters and at any moment of time.

Figure 12. Experimental validation for experiments 3 and 4 at $t=40s$ demonstrating ability to spatially resolve heat flux. (a) Schematic of active heaters and observed temperature map at $t = 40s$. (b) Imposed and retrieved heat fluxes in each heater at $t=40s$.

We performed an uncertainty analysis based on the uncertainty of the inputs to this method. The uncertainty analysis was performed following the GUM-ISO uncertainty procedure [27]. The uncertainty propagation of the non-linear problem was evaluated using the sensitivity method where the standard deviation of each relevant measured quantity is implemented in the calculation of the heat flux and the variation in the heat flux result is assumed to be the uncertainty of the measured/computed heat flux.

For this case, we consider the uncertainty in the thermal properties of the different materials that compose the microchip with the heaters, in the thickness of the materials ($50 \mu m$), and finally in the measured temperatures ($\pm 2K$, after the calibration of the thermocouples and the IR camera). Combining linearly all the contributions to the uncertainty, we observe that the uncertainty in temperature dominates the overall uncertainty. Based on the experimental setup, the overall uncertainty of the new non-linear non-iterative methodology is 7.1% for evaluating the value of predicted heat flux, as shown in Table 1.

Table 1. Uncertainty analysis of the heat flux computation using the non-linear inverse method.

Quantity	Material	Absolute input uncertainty	Uncertainty in %	Variation in heat flux %	Sensitivity
Temperature [K]	-	2.0	0.64	6.35	9.98
k [W/(m K)]	Silicon	10	7.69	-0.15	-0.02
ρ [kg/m ³]	Silicon	10	0.43	0.14	0.32
c_p [J/(kg K)]	Silicon	7	0.99	0.30	0.30
k [W/(m K)]	Polysilicon	10	10.00	-1.66	-0.17
ρ [kg/m ³]	Polysilicon	10	0.43	0.09	0.21
c_p [J/(kg K)]	Polysilicon	7	1.03	0.15	0.15
Thickness [μ m]	Silicon	50	5.00	1.97	0.39
Thickness [μ m]	Polysilicon	50	10.00	1.97	0.20
Overall Uncertainty in heat flux calculation				7.14	-

When comparing the heat flux extracted from our inverse method to that measured directly in the measurement rig, we must also consider the uncertainty in the power measurements. Specifically, the uncertainty of the experimentally measured heat flux is 4.6% as evaluated given the uncertainty in the voltmeter and sourcemeter measurements. Table 2 shows the uncertainty associated to the power computed in each one of the heaters that we used as heat source during the different experiments.

Table 2. Uncertainty calculation of the power in the experiments.

Quantity	Absolute uncertainty	Uncertainty in %	Variation of power relative to mean in %	Sensitivity
Voltage [V]	0.005	0.152	4.591	30.30
Current [A]	0.00001	0.002	0.278	166.67
Overall uncertainty in power calculation			4.60	

CONCLUSIONS

This manuscript presented a new inverse heat transfer methodology, that combines the Digital Filter Method with a non-linear approach to compute the sensitivity coefficients with respect to the heat flux and a correction for convective heat transfer, that only depends on the gas to wall temperature difference. The methodology was validated using numerical and experimental tests, considering only conduction and also fully conjugate heat transfer analysis. The Matlab routine is coupled to two different commercial solvers, COMSOL Multiphysics and ANSYS Fluent. The experiment was performed using an infrared microscope, that enabled tracking the temperature on the surface of a microchip equipped with 25 heaters, in a temperature-controlled environment. The measured temperature map was

the input of the inverse methodology, to retrieve the heat flux that generated such temperature distribution. COMSOL was used to model conduction within the chip with limited natural convection boundary conditions, whereas ANSYS Fluent was used for forced convection cases with conjugate heat transfer models including both the solid and fluid. Both type of validations exhibited a good agreement, the magnitude, location and time distribution of the heat flux for the different cases was predicted with good accuracy using experimental data obtained with an infrared microscope.

This agreement of the retrieved and the imposed heat flux confirms the ability of the new method to predict the temporal and spatial boundary conditions, taking into account the temperature varying properties of the materials and convective boundaries that introduce non-linearities in the heat flux inverse calculation. This physics-based methodology can be expanded to other applications beyond micro-electronics, providing good results if the physics are correctly modelled. It can be applied to other types of boundary conditions such as radiation.

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NOMENCLATURE

C_p	=	Heat capacity [J/(kg K)]
F	=	Temperature factor
H	=	Hessian matrix
k	=	Conductivity [W/(m K)]
T	=	Calculated temperature [K]
q	=	Heat flux [W/m ²]
X	=	Sensitivity coefficient matrix
Y	=	Measured temperature [K]

Greek symbols

α	=	Regularization parameters
ρ	=	Density [kg/m ³]

Subscripts

i	=	Particular time step
j	=	Particular space location
m	=	Total number of temperature measurements
n	=	Total number of time steps
p	=	Total number of heat sources

Acronyms

<i>BFGS</i>	=	Broyden-Fletcher-Goldfarb-Shanno method
<i>CGM</i>	=	Conjugate Gradient Method

DFM = Digital Filter Method
RTD = Resistance Temperature Detector

REFERENCES

- [1] Hadamard, Jacques (1902). “*Sur les problèmes aux dérivées partielles et leur signification physique*”. Princeton University, Bulletin. pp. 49–52.
- [2] Stolz, G., Jr., “*Numerical Solutions to an Inverse Problem of Heat Conduction for Simple Shapes*”, J. Heat transfer 82, 20-26, (1960).
- [3] CR. Wylie. (4th Edn), Advanced Engineering Mathematics, McGraw-Hill Kogakusha, Tokio (1975).
- [4] Beck, J. V., Blackwell, B., St. Clair, C. R. Jr., “*Inverse heat Conduction. Ill-Posed Problems*”. A Wiley-Interscience Publication, N. Y., 308 pp.
- [5] R. V. Churchill, "Modern Operational Mathematics in Engineering." McGraw-Hill Book Company, Inc., New York, N. Y., 1944, pp. 214-216.
- [6] J. Blum, W. Marquardt, “*An optimal solution to inverse heat conduction problems based on frequency domain interpretation and observers*”, Numer. Heat Transfer Part B Fundam. 32 (4) (1997) 453–478.
- [7] K.D. Cole, J.V. Beck, A. Haji-Sheikh, B. Litkouhi, “*Heat conduction using green’s functions*,” Series in Computational and Physical Processes in Mechanics and Thermal Sciences, Taylor & Francis Group, 2010.
- [8] Fernandes, A. P., dos Santos, M. B., & Guimarães, G. (2015). “*An analytical transfer function method to solve inverse heat conduction problems*”. Applied Mathematical Modelling, 39(22), 6897-6914.
- [9] Alifanov, O. M. “*Inverse heat transfer problems*”. Springer Science & Business Media, 2012.
- [10] Beck, J. V. and Arnold K. J., *Parameter Estimation in Engineering and Science*, Wiley, New York, 1977.
- [11] Ozisik, M. Necati, Orlande R. B. Helcio, “*Inverse heat transfer: fundamentals and applications*. CRC Press, 2000.
- [12] Alifanov, O. M., “*Solution of an Inverse Problem of Heat-Conduction by Iterative Methods*”, J. Eng. Phys., 26(4), 471-476, 1974.
- [13] Tikhonov, A. N., “*Inverse Problems in Heat Conduction*”, J. Eng. Phys., 29(1), 816-820, 1975.
- [14] Marquardt, D. W., “*An Algorithm for Least Squares Estimation of Nonlinear Parameters*”, J. Soc. Ind. Appl. Math, 11, 431-441, 1963.
- [15] Beck, J. V., “*Criteria for comparison of methods of Solution of the Inverse Heat Conduction Problem*”, Nuclear Engineering and Design, 53, 11-22, 1979.

- [16] Levenberg, K., "A Method for the Solution of Certain Non-linear Problems in Least-Squares", Quart. Appl. Math, 2, 164-1 68, 1944.
- [17] H. Najafi, K.A. Woodbury, J.V. Beck, "A filter based solution for inverse heat conduction problems in multi-layer mediums", Int. J. Heat Mass Transfer, 83, (April 2015) 710–720.
- [18] H. Najafi, K.A. Woodbury, J.V. Beck, "Real time solution for inverse heat conduction problems in a two-dimensional plate with multiple heat fluxes at the surface", Int. J. Heat Mass Transfer, 91, (September 2015) 1148-1156.
- [19] Cuadrado, D.G., Marconnet, A. and Paniagua, G., 2018. "Inverse Conduction Heat Transfer and Kriging Interpolation Applied to Temperature Sensor Location in Microchips," Journal of Electronic Packaging, 140(1), p.010905.
- [20] Bialecki, R. A., Divo, E., Kassab, A. J., Ait Maalem Lahcen, R., "Explicit calculation of smoothed sensitivity coefficients for linear problems", International Journal for Numerical Methods In Engineering, 2003; 57:143–167. DOI: 10.1002/nme.671
- [21] Tikhonov, A. N. and Arsenin, V. Y., "Solution of Ill-Posed Problems", Winston & Sons, Washington, DC, 1977.
- [22] Tikhonov, A. N., "Solution of Incorrectly Formulated Problems and the Regularization Method", Soviet Math. Dokl. , 4(4), 1035- 1038, 1963.
- [23] Tikhonov, A. N., "Regularization of Incorrectly Posed Problems", Soviet Math. Dokl. , 4(6), 1624- 1627, 1963.
- [24] Timans, P. J., "Emissivity of silicon at elevated temperatures", Journal of Applied Physics 74, 6353 (1993); doi:10.1063/1.355159
- [25] Kaipio, J., Somersalo, E., "Statistical inverse problems: Discretization, model reduction and inverse crimes" , Journal of Computational and Applied Mathematics, Volume 198, Issue 2, 2007, 493-504, ISSN 0377-0427, doi:10.1016/j.cam.2005.09.027.
- [26] Cuadrado, D. G., Lozano, F., and Paniagua, G.. "Experimental Demonstration of Inverse Heat Transfer Methodologies for Turbine Applications." Proceedings of the ASME Turbo Expo 2019: Turbomachinery Technical Conference and Exposition, Volume 6, Phoenix, Arizona, USA, June 17–21, 2019. V006T05A018. ASME, doi:10.1115/GT2019-91105.
- [27] JCGM 100:2008 GUM 1995 with minor corrections "Evaluation of measurement data - Guide to the expression of uncertainty in measurement", Joint Committee for Guides in Metrology, 2008.

APPENDIX

1. Direct Heat Transfer Model Equations

As specified in the main manuscript there are two models that have been developed: a direct model to solve the heat transfer problem starting from the boundary conditions and an inverse model to solve the heat transfer model starting from its solution (to get the boundary conditions).

The direct model, developed in COMSOL Multiphysics solves the 3D unsteady-state energy equation for a solid.

$$c\rho \frac{\delta T}{\delta t} = \frac{\delta}{\delta x} \left(k \frac{\delta T}{\delta x} \right) + \frac{\delta}{\delta y} \left(k \frac{\delta T}{\delta y} \right) + \frac{\delta}{\delta z} \left(k \frac{\delta T}{\delta z} \right) + q_{gen}$$

Where c is the specific heat of the material, ρ is the density of the material, T is temperature, t is time, x, y , & z are distances in Cartesian coordinates, and q_{gen} is the rate of heat generated per unit volume.

The boundary conditions applied to each case are specified in the main manuscript. In the calculation of the sensitivity coefficients we imposed heat generation in one of the central heaters:

$$q_{pulse} = 100 \text{ W/m}^3$$

This pulse is imposed at time $t=0$ s and the sensitivity coefficient is obtained

In the numerical validation, we imposed a sinusoidal heat generation in one of the heaters:

$$q_{gen} = 20 - (20 \cdot \sin(3 \cdot i_t)) \frac{W}{m^3} \text{ where } 0 \leq i_t \leq \pi$$

Additionally, for the case of the conjugate heat transfer method, the model solves the heat conduction equation in the solid and the Navier-Stokes equations in the fluid domain with $k-\omega$ transitional SST to model near wall turbulence. In the interface between solid and fluid there is no boundary condition imposed. They are embedded in the ANSYS model.

Continuity Equation

$$\frac{D\rho}{Dt} + \rho \frac{\partial U_i}{\partial x_i} = 0$$

Momentum Equation

$$\underbrace{\rho \frac{\partial U_j}{\partial t}}_I + \underbrace{\rho U_i \frac{\partial U_j}{\partial x_i}}_{II} = - \underbrace{\frac{\partial P}{\partial x_j}}_{III} - \underbrace{\frac{\partial \tau_{ij}}{\partial x_i}}_{IV} + \underbrace{\rho g_j}_V$$

Where

$$\tau_{ij} = -\mu \left(\frac{\partial U_j}{\partial x_i} + \frac{\partial U_i}{\partial x_j} \right) + \frac{2}{3} \delta_{ij} \mu \frac{\partial U_k}{\partial x_k}$$

- I: Local change with time
 - II: Momentum convection
 - III: Surface force
 - IV: Molecular-dependent momentum exchange (diffusion)
 - V: Mass force
- Energy Equation**

$$\underbrace{\rho c_\mu \frac{\partial T}{\partial t}}_I + \underbrace{\rho c_\mu U_i \frac{\partial T}{\partial x_i}}_{II} = - \underbrace{P \frac{\partial U_i}{\partial x_i}}_{III} + \underbrace{\lambda \frac{\partial^2 T}{\partial x_i^2}}_{IV} - \underbrace{\tau_{ij} \frac{\partial U_j}{\partial x_i}}_V$$

- I : Local energy change with time
- II: Convective term
- III: Pressure work
- IV: Heat flux (diffusion)
- V: Irreversible transfer of mechanical energy into heat

2. Inverse Heat Transfer Model Equations

The inverse model, developed in MatLab, solves the linearized heat conduction equation based in the Levenberg-Marquardt method, specified in the main part of the manuscript”

$$q_c = [X^T X + \alpha_t H_t^T H_t + \alpha_s H_s^T H_s]^{-1} X^T T$$

In this case, there are no thermal boundary conditions q_c applied to this equation, since we are looking for the boundary conditions solving this equation. The inputs of this equation consist on the temperature maps provided by the experiment in the experimental validation and for the direct model in the numerical validation.

3. Temperature Dependent Thermal Properties

The temperature dependence, as explained in the manuscript, is provided by the natural convection boundary conditions and the temperature dependent thermal properties. The silicon layers conductivity was modelled following the equation:

$$k(T) = \frac{1}{-2.2 \cdot 10^{-11} \cdot T^3 + 9 \cdot 10^{-8} \cdot T^2 - 1 \cdot 10^{-5} \cdot T + 0.014}$$

Where T is the temperature in Kelvin.