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Inverse Heat Conduction Problems

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1. Introduction

In the heat conduction problems if the heat flux and/or temperature histories at the surface of a solid body are known as functions of time, then the temperature distribution can be found. This is termed as a direct problem. However in many heat transfer situations, the surface heat flux and temperature histories must be determined from transient temperature measurements at one or more interior locations. This is an inverse problem. Briefly speaking one might say the inverse problems are concerned with determining causes for a desired or an observed effect.

The concept of an inverse problem have gained widespread acceptance in modern applied mathematics, although it is unlikely that any rigorous formal definition of this concept exists. Most commonly, by inverse problem is meant a problem of determining various quantitative characteristics of a medium such as density, thermal conductivity, surface loading, shape of a solid body etc., by observation over physical fields in the medium or – in other words - a general framework that is used to convert observed measurements into information about a physical object or system that we are interested in. The fields may be of natural appearance or specially induced, stationary or depending on time, (Bakushinsky & Kokurin, 2004).

Within the class of inverse problems, it is the subclass of indirect measurement problems that characterize the nature of inverse problems that arise in applications. Usually measurements only record some indirect aspect of the phenomenon of interest. Even if the direct information is measured, it is measured as a correlation against a standard and this correlation can be quite indirect. The inverse problems are difficult because they usually are extremely sensitive to measurement errors. The difficulties are particularly pronounced as one tries to obtain the maximum of information from the input data.

A formal mathematical model of an inverse problem can be derived with relative ease. However, the process of solving the inverse problem is extremely difficult and the so-called exact solution practically does not exist. Therefore, when solving an inverse problem the approximate methods like iterative procedures, regularization techniques, stochastic and system identification methods, methods based on searching an approximate solution in a subspace of the space of solutions (if the one is known), combined techniques or straight numerical methods are used.

2. Well-posed and ill-posed problems

The concept of well-posed or correctly posed problems was introduced in (Hadamard, 1923). Assume that a problem is defined as
where \( u \in U, g \in G \), \( U \) and \( G \) are metric spaces and \( A \) is an operator so that \( AU \subset G \). In general \( u \) can be a vector that characterizes a model of phenomenon and \( g \) can be the observed attribute of the phenomenon.

A well-posed problem must meet the following requirements:
- the solution of equation (1) must exist for any \( g \in G \),
- the solution of equation (1) must be unique,
- the solution of equation (1) must be stable with respect to perturbation on the right-hand side, i.e. the operator \( A^{-1} \) must be defined throughout the space \( G \) and be continuous.

If one of the requirements is not fulfilled the problem is termed as an ill-posed. For ill-posed problems the inverse operator \( A^{-1} \) is not continuous in its domain \( AU \subset G \) which means that the solution of the equation (1) does not depend continuously on the input data \( g \in G \), (Kurpisz & Nowak, 1995; Hohage, 2002; Grysa, 2010). In general we can say that the (usually approximate) solution of an ill-posed problem does not necessarily depend continuously on the measured data and the structure of the solution can have a tenuous link to the measured data. Moreover, small measurement errors can be the source for unacceptable perturbations in the solution. The best example of the last statement is numerical differentiation of a solution of an inverse problem with noisy input data. Some interesting remarks on the inverse and ill-posed problems can be found in (Anderssen, 2005).

Some typical inverse and ill-posed problems are mentioned in (Tan & Fox, 2009).

### 3. Classification of the inverse problems

Engineering field problems are defined by governing partial differential or integral equation(s), shape and size of the domain, boundary and initial conditions, material properties of the media contained in the field and by internal sources and external forces or inputs. As it has been mentioned above, if all of this information is known, the field problem is of a direct type and generally considered as well posed and solvable. In the case of heat conduction problems the governing equations and possible boundary and initial conditions have the following form:

\[
p c \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + \dot{Q}, \quad (x,y,z) \in \Omega \subset R^3, \quad t \in (0, t_f], \tag{2}
\]

\[
T(x,y,z,t) = T_b(x,y,z,t) \quad \text{for} \quad (x,y,z,t) \in S_D, \quad t \in (0, t_f], \tag{3}
\]

\[
-k \frac{\partial T(x,y,z,t)}{\partial n} = q_b(x,y,z,t) \quad \text{for} \quad (x,y,z,t) \in S_N, \quad t \in (0, t_f], \tag{4}
\]

\[
-k \frac{\partial T(x,y,z,t)}{\partial n} = h_c \left(T(x,y,z,t) - T_c(x,y,z,t)\right) \quad \text{for} \quad (x,y,z,t) \in S_R, \quad t \in (0, t_f], \tag{5}
\]

\[
T(x,y,z,0) = T_0(x,y,z) \quad \text{for} \quad (x,y,z) \in \Omega, \tag{6}
\]
where $\nabla = (\partial / \partial x, \partial / \partial y, \partial / \partial z)$ stands for gradient differential operator in 3D; $\rho$ denotes density of mass, [kg/m$^3$]; $c$ is the constant-volume specific heat, [J/kg K]; $T$ is temperature, [K]; $k$ denotes thermal conductivity, [W/m K]; $\dot{Q}_s$ is the rate of heat generation per unit volume, [W/m$^3$], frequently termed as source function; $\partial / \partial \mathbf{n}$ means differentiation along the outward normal; $\mathbf{h}$ denotes the heat transfer coefficient, [W/m$^2$ K]; $T_b$, $\phi_b$ and $T_0$ are given functions and $T_e$ stands for environmental temperature, $t_f$ – final time. The boundary $\partial \Omega$ of the domain $\Omega$ is divided into three disjoint parts denoted with subscripts $D$ for Dirichlet, $N$ for Neumann and $R$ for Robin boundary condition; $S_D \cup S_N \cup S_R = \partial \Omega$.

Moreover, it is also possible to introduce the fourth-type or radiation boundary condition, but here this condition will not be dealt with.

The equation (2) with conditions (3) to (6) describes an initial-boundary value problem for transient heat conduction. In the case of stationary problem the equation (2) becomes a Poisson equation or – when the source function $\dot{Q}_s$ is equal to zero – a Laplace equation.

Broadly speaking, inverse problems may be subdivided into the following categories: inverse conduction, inverse convection, inverse radiation and inverse phase change (melting or solidification) problems as well as all combination of them (Özisik & Orlande, 2000). Here we have adopted classification based on the type of causal characteristics to be estimated:

1. Boundary value determination inverse problems,
2. Initial value determination inverse problems,
3. Material properties determination inverse problems,
4. Source determination inverse problems
5. Shape determination inverse problems.

3.1 Boundary value determination inverse problems

In this kind of inverse problem on a part of a boundary the condition is not known. Instead, in some internal points of the considered body some results of temperature measurements or anticipated values of temperature or heat flux are prescribed. The measured or anticipated values are called internal responses. They can be known on a line or surface inside the considered body or in a discrete set of points. If the internal responses are known as values of heat flux, on a part of the boundary a temperature has to be known, i.e. Dirichlet or Robin condition has to be prescribed. In the case of stationary problems an inverse problem for Laplace or Poisson equation has to be solved. If the temperature field depends on time, then the equation (2) becomes a starting point. The additional condition can be formulated as

$$T(x,y,z,t) = T_{a}(x,y,z,t) \text{ for } (x,y,z) \in L \subset \Omega, \ t \in (0, t_f]$$

or

$$T(x_i,y_i,z_i,t_k) = T_{ik} \text{ for } (x_i,y_i,z_i) \in \Omega, \ t_k \in (0, t_f], i=1,2,\ldots, I; k=1,2,\ldots, K$$

with $T_a$ being a given function and $T_{ik}$ known from e.g. measurements. As examples of such problems can be presented papers (Reinhardt et al., 2007; Soti et al., 2007; Ciałkowski & Grysa, 2010) and many others.
3.2 Initial value determination inverse problems

In this case an initial condition is not known, i.e. in the condition (6) the function $T_0$ is not known. In order to find the initial temperature distribution a temperature field in the whole considered domain for fixed $t>0$ has to be known, i.e. instead of the condition (6) a condition like

$$T(x,y,z,t_m) = T_0(x,y,z) \quad \text{for} \quad (x,y,z) \in \Omega \quad \text{and} \quad t_m \in (0, t]$$

has to be specified, compare (Yamamoto & Zou, 2001; Masood et al., 2002). In some papers instead of the condition (9) the temperature measurements on a part of the boundary are used, see e.g. (Pereverzyev et al., 2005).

3.3 Material properties determination inverse problems

Material properties determination makes a wide class of inverse heat conduction problems. The coefficients can depend on spatial coordinates or on temperature. Sometimes dependence on time is considered. In addition to the coefficients mentioned in part 3 also the thermal diffusivity, $a = k / \rho c$, [m/s$^2$] is the one frequently being determined. In the case when thermal conductivity depends on temperature, Kirchhoff substitution is useful, (Ciakowski & Grysa, 2010a). Also in the case of material properties determination some additional information concerning temperature and/or heat flux in the domain has to be known, usually the temperature measurements taken at the interior points, compare (Yang, 1998; Onyango et al., 2008; Hożejowski et al., 2009).

3.4 Source determination inverse problems

In the case of source determination, $Q_i$, one can identify intensity of the source, its location or both. The problems are considered for steady state and for transient heat conduction. In many cases as an extra condition the temperature data are given at chosen points of the domain $\Omega$, usually as results of measurements, see condition (8). As an additional condition can be also adopted measured or anticipated temperature and heat flux on a part of the boundary. A separate class of problems are those concerning moving sources, in particular those with unknown intensity. Some examples of such problems can be found in papers (Grysa & Maciejewska, 2005; Ikehata, 2007; Jin & Marin, 2007; Fan & Li, 2009).

3.5 Shape determination inverse problems

In such problems, in contrast to other types of inverse problems, the location and shape of the boundary of the domain of the problem under consideration is unknown. To compensate for this lack of information, more information is provided on the known part of the boundary. In particular, the boundary conditions are overspecified on the known part, and the unknown part of the boundary is determined by the imposition of a specific boundary condition(s) on it.

The shape determination inverse problems can be subdivided into two class. The first one can be considered as a design problem, e.g. to find such a shape of a part of the domain boundary, for which the temperature or heat flux achieves the intended values. The problems become then extremely difficult especially in the case when the boundary is multiply connected.
The second class is termed as Stefan problem. The Stefan problem consists of the determination of temperature distribution within a domain and the position of the moving interface between two phases of the body when the initial condition, boundary conditions and thermophysical properties of the body are known. The inverse Stefan problem consists of the determination of the initial condition, boundary conditions and thermophysical properties of the body. Lack of a portion of input data is compensated with certain additional information.

Among inverse problems, inverse geometric problems are the most difficult to solve numerically as their discretization leads to system of non-linear equations. Some examples of such problems are presented in (Cheng & Chang, 2003; Dennis et al., 2009; Ren, 2007).

4. Methods of solving the inverse heat conduction problems

Many analytical and semi-analytical approaches have been developed for solving heat conduction problems. Explicit analytical solutions are limited to simple geometries, but are very efficient computationally and are of fundamental importance for investigating basic properties of inverse heat conduction problems. Exact solutions of the inverse heat conduction problems are very important, because they provide closed form expressions for the heat flux in terms of temperature measurements, give considerable insight into the characteristics of inverse problems, and provide standards of comparison for approximate methods.

4.1 Analytical methods of solving the steady state inverse problems

In 1D steady state problems in a slab in which the temperature is known at two or more location, thermal conductivity is known and no heat source acts, a solution of the inverse problem can be easily obtained. For this situation the Fourier's law, being a differential equation to integrate directly, indicates that the temperature profile must be linear, i.e.

\[ T(x) = ax + b = -qx / k + T_{\text{con}}, \]  

(10)

with two unkowns, \( q \) (the steady-state heat flux) and \( T_{\text{con}} \) (a constant of integration). Suppose the temperature is measured at \( J \) locations, \( \{x_1, x_2, ..., x_J\} \), below the upper surface (with \( x \)-axis directed from the surface downward) and the experimental temperature measurements are \( Y_j, j = 1,2, ..., J \). The steady-state heat flux and the integration constant can be calculated by minimizing the least square error between the computed and experimental temperatures. In order to generalize the analysis, assume that some of the sensors are more accurate than others, as indicated by the weighting factors, \( w_j, j = 1,2, ..., J \). A weighted least square criterion is defined as

\[ I = \sum_{j=1}^{J} w_j^2 \left( Y_j - T(x_j) \right)^2. \]  

(11)

Differentiating equation (11) with respect to \( q \) and \( T_{\text{con}} \) gives

\[ \sum_{j=1}^{J} w_j^2 \left( Y_j - T(x_j) \right) \frac{\partial T(x_j)}{\partial q} = 0 \quad \text{and} \quad \sum_{j=1}^{J} w_j^2 \left( Y_j - T(x_j) \right) \frac{\partial T(x_j)}{\partial T_{\text{con}}} = 0. \]  

(12)
Equations (12) involve two sensitivity coefficients which can be evaluated from (10), \( \partial T(x_j)/\partial q = -x_j/k \) and \( \partial T(x_j)/\partial T_{\text{con}} = 1, j = 1,2,\ldots,J \), (Beck et al., 1985). Solving the system of equations (12) for the unknown heat flux gives

\[
q = -k \left\{ \sum_{j=1}^{J} w_j^2 \left( \sum_{j=1}^{J} w_j^2 x_j \right) - \left( \sum_{j=1}^{J} w_j^2 x_j \right) \right\}. 
\]

(13)

Note, that the unknown heat flux is linear in the temperature measurements.

Constants \( a \) and \( b \) in equation (10) could be developed by fitting a weighted least square curve to the experimental temperature data. Differentiating the curve according to Fourier's a law leads also to formula (13).

In the case of 2D and 3D steady state problems with constant thermophysical properties, the heat conduction equation becomes a Poisson equation. Any solution of the homogeneous (Laplace) equation can be expressed as a series of harmonic functions. An approximate solution, \( u \), of an inverse problem can be then presented as a linear combination of a finite number of polynomials or harmonic functions plus a particular solution of the Poisson equation:

\[
u = \sum_{k=1}^{K} \alpha_k H_k + T^{\text{part}}
\]

(14)

where \( H_k \)'s stand for harmonic functions, \( \alpha_k \) denotes the \( k \)-th coefficient of the linear combination of the harmonic functions, \( k = 1,2,\ldots,K \), and \( T^{\text{part}} \) stands for a particular solution of the Poisson equation. If the experimental temperature measurements \( Y_j, j = 1,2,\ldots,J \), are known, coefficients of the combination, \( \alpha_k \), can be obtained by minimization an objective functional

\[
I(u) = \int_{\Omega} \left( \nabla^2 u - \bar{Q}_t \right)^2 d\Omega + \int_{S} \left( u - T_y \right)^2 dS + \int_{S} \left( k \frac{\partial u}{\partial n} + q_b \right)^2 dS \]

\[
+ \int_{S} \left( k \frac{\partial u}{\partial n} + h_v \frac{\partial u}{\partial n} - h_T T_y \right)^2 dS + \sum_{j=1}^{J} \left( Y_j - u(x_j) \right)^2
\]

(15)

where \( x_j \in \Omega \); \( w_1, w_2, w_3 \) - weights. Note that for harmonic functions the first integral vanishes.

### 4.2 Burggraf solution

Considering 1D transient boundary value inverse problem in a flat slab Burggraf obtained an exact solution in the case when the time-dependant temperature response was known at one internal point, (Burggraf, 1964). Assuming that \( T(x^*,t) = T^*(t) \) and \( q(x^*,t) = q^*(t) \) are known and are of class \( C^\infty \) in the considered domain, Burggraf found an exact solution to the inverse problem for a flat slab, a sphere and a circular cylinder in the following form:
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\[
T(x,t) = \sum_{n=0}^{\infty} \left[ f_n(x) \frac{d^n T^*}{dt^n} - \frac{1}{a} g_n(x) \frac{d^n q^*}{dt^n} \right].
\]  

(16)

with \( a \) standing for thermal diffusivity, \( a = k / \rho c \), \([\text{m/s}]^2\]. The functions \( f_n(x) \) and \( g_n(x) \)
have to fulfill the conditions

\[
\begin{align*}
\frac{d^2 f_0}{dx^2} &= 0, & \frac{d^2 f_n}{dx^2} &= \frac{1}{a} f_{n-1}, & \frac{d^2 g_0}{dx^2} &= 0, & \frac{d^2 g_n}{dx^2} &= \frac{1}{a} g_{n-1}, & n &= 1, 2, \ldots; \\
f_0(x^*) &= 1, & f_n(x^*) &= 0, & \left. \frac{df_n}{dx} \right|_{x^*} &= 0, & n &= 0, 1, \ldots; \\
g_0(x^*) &= 0, & \left. \frac{dg_n}{dx} \right|_{x^*} &= 1, & g_n(x^*) &= 0, & \left. \frac{dg_n}{dx} \right|_{x^*} &= 0, & n &= 1, 2, \ldots.
\end{align*}
\]

It is interesting that no initial condition is needed to determine the solution. This follows from the assumption that the functions \( T^*(t) \) and \( q^*(t) \) are defined for \( t \in [0, \infty) \).

The solutions of 1D inverse problems in the form of infinite series or polynomials was also proposed in (Kover'yanov, 1967) and in other papers.

4.3 Laplace transform approach

The Laplace transform approach is an integral technique that replaces time variable and the time derivative by a Laplace transform variable. This way in the case of 1D transient problems, the partial differential equation converts to the form of an ordinary differential equation. For the latter it is not difficult to find a solution in a closed form. However, in the case of inverse problems inverting of the obtained solutions to the time-space variables is practically impossible and usually one looks for approximate solutions, (Woo & Chow, 1981; Soti et al., 2007; Ciałkowski & Grysa, 2010). The Laplace transform is also useful when 2D inverse problems are considered (Monde et al., 2003)

The Laplace transform approach usually is applied for simple geometry (flat slab, halfspace, circular cylinder, a sphere, a rectangle and so on).

4.4 Trefftz method

The method known as “Trefftz method” was firstly presented in 1926, (Trefftz, 1926). In the case of any direct or inverse problem an approximate solution is assumed to have a form of a linear combination of functions that satisfy the governing partial linear differential equation (without sources). The functions are termed as Trefftz functions or T-functions. In the space of solutions of the considered equation they form a complete set of functions. The unknown coefficients of the linear combination are then determined basing on approximate fulfillment the boundary, initial and other conditions (for instance prescribed at chosen points inside the considered body), finally having a form of a system of algebraic equations (Ciałkowski & Grysa, 2010a).

T-functions usually are derived for differential equation in dimensionless form. The equation (2) with zero source term and constant material properties can be expressed in dimensionless form as follows:
where $\xi$ stands for dimensionless spatial location and $\tau = k/\rho c$ denotes dimensionless time (Fourier number). In further consideration we will use notation $x = (x, y, z)$ and $t$ for dimensionless coordinates.

For dimensionless heat conduction equation in 1D the set of $T$-functions read

$$v_\alpha(x,t) = \sum_{n=0}^{[n/2]} x^{n-2k} \frac{k^k}{(n-2k)!k!} , \quad n = 0,1,...$$  \hspace{1cm} (17)

where $[n/2] = \text{floor}(n/2)$ stands for the greatest previous integer of $n/2$. T-functions in 2D are the products of proper T-functions for the 1D heat conduction equations:

$$v_m(x,y,t) = v_{m-1}(x,t)v_y(y,t) , \quad n = 0,1,... \hspace{0.5cm} k = 0,...,n ; \hspace{0.5cm} m = \frac{n(n+1)}{2} + k$$  \hspace{1cm} (18)

The 3D T-functions are built in a similar way.

Consider an inverse problem formulated in dimensionless coordinates as follows:

$$\nabla^2 T = \frac{\partial T}{\partial \tau} \hspace{1cm} \text{in} \hspace{0.5cm} \Omega \times (0,\tau_f),$$

$$T = g_1 \hspace{1cm} \text{on} \hspace{0.5cm} S_D \times (0,\tau_f),$$

$$\frac{\partial T}{\partial n} = g_2 \hspace{1cm} \text{on} \hspace{0.5cm} S_N \times (0,\tau_f),$$

$$\frac{\partial T}{\partial n} + \text{Bi} \frac{T}{T} = \text{Big}_3 \hspace{1cm} \text{on} \hspace{0.5cm} S_R \times (0,\tau_f),$$

$$T = g_4 \hspace{1cm} \text{on} \hspace{0.5cm} S_{\text{int}} \times T_{\text{int}},$$

$$T = h \hspace{1cm} \text{on} \hspace{0.5cm} \Omega \hspace{0.5cm} \text{for} \hspace{0.5cm} t = 0,$$

where $S_{\text{int}}$ stands for a set of points inside the considered region, $T_{\text{int}} \subset (0,\tau_f)$ is a set of moments of time, the functions $g_i$, $i=1,2,3,4$ and $h$ are of proper class of differentiability in the domains in which they are determined and $S_D \cup S_N \cup S_R = \partial \Omega$. $\text{Bi}=h\rho c/k$ denotes the Biot number (dimensionless heat transfer coefficient) and $l$ stands for characteristic length. The sets $S_{\text{int}}$ and $T_{\text{int}}$ can be continuous (in the case of anticipated or smoothed or described by continuous functions input data) or discrete. Assume that $g_1$ in not known and $g_4$ describes results of measurements on $S_{\text{int}} \times T_{\text{int}}$. An approximate solution of the problem is expressed as a linear combination of the T-functions

$$T \approx u = \sum_{k=1}^{K} \alpha_k \theta_k$$  \hspace{1cm} (21)

with $\theta_k$ standing for T-functions. The objective functional can be written down as
\[ I(u) = \int_{S_{\text{int}} \times (0, \tau_f)} (\partial u / \partial n - g_2)^2 \, dSdt \]
\[ + \int_{S_x \times (0, \tau_f)} (\partial u / \partial n + B_1 u - B_2 g_1)^2 \, dSdt \]
\[ + \int_{S_{\text{int}} \times (0, \tau_f)} (u - h)^2 \, dSdt + \int\left(\nabla^2 \partial / \partial t\right)u \, d\Omega \]
\[ \text{In the contrary to the formula (15), the integral containing residuals of the governing equation fulfills,} \]
\[ \int\left((\nabla^2 \partial / \partial t)u\right)^2 \, d\Omega dt, \text{ does not appear here because } u, \text{ as a linear combination of T-functions, satisfies the equation (20). Minimization of the functional } I(u) \]
\[ \text{(being in fact a function of } K \text{ unknown coefficients, } \alpha_1, \ldots, \alpha_K \text{) leads to a system of } K \]
\[ \text{algebraic equations for the unknowns. The solution of this system leads to an approximate solution, (21), of the considered problem. Hence, for } (x, \tau) \in S_{\text{int}} \times (0, \tau_f) \text{ one obtains approximate form of the functions } g_1. \]

It is worth to mention that approximate solution of the considered problem can also be obtained in the case when, for instance, the function \( h \) is unknown. In the formula (21) the last term is then omitted, but the minimization of the functional \( I(u) \) can be done. The final result has physical meaning, because the approximate solution (21) consists of functions satisfying the governing partial differential equation.

The greater the number of T-functions in (21), the better the approximation of the solutions takes place. However, with increasing \( K \), conditioning of the algebraic system of equation that results from minimization of \( I(u) \) can become worse. Therefore, the set \( S_{\text{int}} \) has to be chosen very carefully.

Since the system of algebraic equations for the whole domain may be ill-conditioned, a finite element method with the T-functions as base functions is often used to solve the problem.

### 4.5 Function specification method

The function specification method, originally proposed in (Beck, 1962), is particularly useful when the surface heat flux is to be determined from transient measurements at interior locations. In order to accomplish this, a functional form for the unknown heat flux is assumed. The functional form contains a number of unknown parameters that are estimated by employing the least square method. The function specification method can be also applied to other cases of inverse problems, but efficiency of the method for those cases is often not satisfactory.

As an illustration of the method, consider the 1D problem
\[ a\partial^2 T / \partial x^2 = \partial T / \partial t \quad \text{for } x \in (0, l) \text{ and } t \in (0, t_f], \]
\[ -k \partial T / \partial x = q(t) \quad \text{for } x = 0 \text{ and } t \in (0, t_f], \]
\[ k \partial T / \partial x = f(t) \quad \text{for } x = l \text{ and } t \in (0, t_f], \]

\[ \text{(23)} \]

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\[ T = T_0(x) \quad \text{for } x \in (0, l) \text{ and } t = 0 . \]

For further analysis it is assumed that \( q(t) \) is not known. Instead, some measured temperature histories are given at interior locations:

\[ T(x,i,t_k) = \{ x_j \}_{j=1,...,J} \subset (0,l), \quad \{ t_k \}_{k=1,...,K} \subset (0,t_f) . \]

The heat flux is more difficult to calculate accurately than the surface temperature. When knowing the heat flux it is easy to determine temperature distribution. On the contrary, if the unknown boundary characteristics were assumed as temperature, calculating the heat flux would need numerical differentiating which may lead to very unstable results.

In order to solve the problem, it is assumed that the heat flux is also expressed in discrete form as a stepwise functions in the intervals \((t_{k-1}, t_k)\). It is assumed that the temperature distribution and the heat flux are known at times \(t_{k-1}, t_{k-2}, \ldots \) and it is desired to determine the heat flux \( q_k \) at time \( t_k \). Therefore, the condition (23) can be replaced by

\[ q = -k \frac{\partial T}{\partial x} = \begin{cases} q_k = \text{const} & \text{for } t_{k-1} < t \leq t_k \\ q(t) = \varphi(t) & \text{for } t > t_k \end{cases} \]

Now we assume that the unknown temperature field depends continuously on the unknown heat flux \( q \). Let us denote \( \frac{\partial Z}{\partial T} = \frac{\partial T}{\partial q} \) and differentiate the formulas (23) with respect to \( q \). We arrive to a direct problem

\[ a \frac{\partial^2 Z}{\partial x^2} = \frac{\partial Z}{\partial t} \quad \text{for } x \in (0, l) \text{ and } t \in (0, t_f), \]

\[ -k \frac{\partial Z}{\partial x} = 1 \quad \text{for } x = 0 \text{ and } t \in (0, t_f), \]

\[ k \frac{\partial Z}{\partial x} = 0 \quad \text{for } x = l \text{ and } t \in (0, t_f), \]

\[ Z = 0 \quad \text{for } x \in (0,l) \text{ and } t = 0 . \]

The direct problem (24) can be solved using different methods. Let us introduce now the sensitivity coefficients defined as

\[ Z^k_{i,m} = \frac{\partial T}{\partial q_k} \bigg|_{(x_i,t_m)} = \frac{\partial T(x_i,t_m)}{\partial q_k} . \]

The temperature \( T(x_i,t_m) \) can be expanded in a Taylor series about arbitrary but known values of heat flux \( q_k^* \). Neglecting the derivatives with order higher than one we obtain

\[ T(x_i,t_m) = T(x_i,t_m)^* + \frac{\partial T(x_i,t_m)}{\partial q_k} \bigg|_{q_k=q_k^*} \left( q_k - q_k^* \right) = T(x_i,t_m)^* + Z_{i,m} \left( q_k - q_k^* \right) \]

Making use of (24) and (25), solving (26) for heat flux component \( q_k \) and taking into consideration the temperature history only in one location, \( x_1 \), we arrive to the formula
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\[ q_k = q_k^* \frac{U_{1,k} - T_{1,k}^*}{Z_{1,k}^*}, \quad k = 1, \ldots, K. \]  \hspace{1cm} (27)

In the case when future temperature measurements are employed to calculate \( q_k \), we use another formula (Beck et al., 1985, Kurpisz & Nowak, 1995), namely

\[ q_k = q_k^* \sum_{r=1}^{R} \left( \frac{U_{1,k,r-1} - T_{1,k,r-1}^*}{Z_{1,k,r-1}^*} \right)^2 \sum_{r=1}^{R} (Z_{1,k,r-1}^*)^2 \]  \hspace{1cm} (28)

The case of many interior locations for temperature measurements is described e.g. in (Kurpisz & Nowak, 1995).

The detailed algorithm for 1D inverse problems with one interior point with measured temperature history is presented below:

1. Substitute \( k = 1 \) and assume \( q_k = 0 \) over time interval \( 0 < t \leq t_1 \).
2. Calculate \( T_{1,k,r-1}^* \) for \( r = 1, 2, \ldots, R \), \( R \leq K \), assuming \( q_k = q_{k+1} = \ldots = q_{k+R-1} \); \( T_{1,k,r-1}^* \) should be calculated, employing any numerical method to the following problem: differential equation (23)$_1$, boundary condition (23)$_2$ with \( q_k^* \) instead of \( q(t) \), boundary condition (23)$_3$ and initial condition \( T_{k-1}^* = T_{k-1} \), where \( T_{k-1} \) has been computed for the time interval \( t_{k-2} < t \leq t_{k-1} \) or is an initial condition (23)$_4$ when \( k = 1 \).
3. Calculate \( q_k \) from equation (27) or (28).
4. Determine the complete temperature distribution, using equation (26).
5. Substitute \( k \rightarrow k + 1 \) and \( q_k^* = q_{k-1} \) and repeat the calculations from step 2.

For nonlinear cases an iterative procedure should be involved for step 2 and 3.

### 4.6 Fundamental solution method

The fundamental solution method, like the Trefftz method, is useful to approximate the solution of multidimensional inverse problems under arbitrary geometry. The method uses the fundamental solution of the corresponding heat equation to generate a basis for approximating the solution of the problem.

Consider the problem described by equation (20)$_1$, Dirichlet and Neumann conditions (20)$_2$ and (20)$_3$ and initial condition (20)$_6$. The dimensionless time is here denoted as \( t \). Let \( \Omega \) be a simply connected domain in \( \mathbb{R}^d \), \( d = 2, 3 \). Let \( \{x_i\}_{i=1}^M \subset \Omega \) be a set of locations with noisy measured data \( \tilde{y}_i^{(k)} \) of exact temperature \( T(x, t_i^{(k)}) = Y_i^{(k)}, \quad i = 1, 2, \ldots, M, \quad k = 1, 2, \ldots, J_i \), where \( t_i^{(k)} \in (0, t_f) \) are discrete times. The absolute error between the noisy measurement and exact data is assumed to be bounded for all measurement points at all measured times. The inverse problem is formulated as: reconstruct \( T \) and \( \partial T / \partial n \) on \( S_R \times (0, t_f) \) from (20)$_1$, (20)$_2$, (20)$_3$ and (20)$_6$ and the scattered noisy measurements \( \tilde{y}_i^{(k)} \), \( i = 1, 2, \ldots, M, \quad k = 1, 2, \ldots, J_i \). It is worth to mention that with reconstructed \( T \) and \( \partial T / \partial n \) on \( S_R \times (0, t_f) \) it is easy to identify heat transfer coefficient, \( h \), on \( S_R \).
The fundamental solution of (20) in $\mathbb{R}^d$ is given by

$$ F(x, t) = \frac{1}{(4\pi t)^{d/2}} \exp \left( -\frac{x^2}{4t} \right) H(t) $$

(29)

where $H(t)$ is the Heaviside function. Assuming that $t^* > t_f$ is a constant, the function $\phi(x, t) = F(x, t + t^*)$ is a general solution of (20) in the solution domain $\Omega \times (0, t_f)$.

We denote the measurement points to be $\{(x_j, t_j)\}_{j=1}^m$, $m = \sum_{j=1}^{M} I_j$, so that a point at the same location but with different time is treated as two distinct points. In order to solve the problem one has to choose collocation points. They are chosen as

- $\{(x_j, t_j)\}_{j=m+1}^{m+n}$ on the initial region $\Omega \times \{0\}$,
- $\{(x_j, t_j)\}_{j=m+n+1}^{m+n+p}$ on the surface $S_D \times (0, t_f]$, and
- $\{(x_j, t_j)\}_{j=m+n+p+1}^{m+n+p+q}$ on the surface $S_N \times (0, t_f]$.

Here, $n$, $p$ and $q$ denote the total number of collocation points for initial condition (20)$_6$, Dirichlet boundary condition (20)$_2$, and Neumann boundary condition (20)$_3$, respectively.

To illustrate the procedure of choosing collocation points let us consider an inverse problem in a square (Hon & Wei, 2005): $\Omega = \{(x_1, x_2) : 0 < x_1 < 1, 0 < x_2 < 1\}$, $S_D = \{(x_1, x_2) : x_1 = 1, 0 < x_2 < 1\}$, $S_N = \{(x_1, x_2) : 0 < x_1 < 1, x_2 = 1\}$, $S_R = \partial \Omega \setminus \{S_D \cup S_N\}$.

Distribution of the measurement points and collocation points is shown in Figure 1.

An approximation $\tilde{T}$ to the solution of the inverse problem under the conditions (20)$_2$, (20)$_3$ and (20)$_6$, and the noisy measurements $\tilde{Y}^{(k)}$ can be expressed by the following linear combination:

$$ \tilde{T}(x, t) = \sum_{j=1}^{m+n+p+q} \tilde{\lambda}_j \phi(x - x_j, t - t_j), $$

(30)

where $\phi(x, t) = F(x, t + t^*)$, $F$ is given by (29) and $\tilde{\lambda}_j$ are unknown coefficients to be determined.

For this choice of basis functions $\phi$, the approximated solution $\tilde{T}$ automatically satisfies the original heat equation (20)$_1$. Using the conditions (20)$_2$, (20)$_3$ and (20)$_6$, we then obtain the following system of linear equations for the unknown coefficients $\tilde{\lambda}_j$:

$$ A \tilde{\lambda} = \tilde{b} $$

(31)
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Fig. 1. Distribution of measurement points and collocation points. Stars represent collocation points matching Dirichlet data, squares represent collocation points matching Neumann data, dots represent collocation points matching initial data and circles denotes points with sensors for internal measurement.

where

\[
A = \begin{bmatrix}
\phi(x_i - x_j, t_i - t_j) \\
\frac{\partial \phi}{\partial n}(x_k - x_l, t_k - t_l)
\end{bmatrix}
\]

(32)

and

\[
\vec{b} = \begin{bmatrix}
\tilde{Y}_i \\
h(x_i, t_i) \\
g_1(x_j, t_j) \\
g_2(x_k, t_k)
\end{bmatrix}
\]

(33)

where \( i = 1, 2, \ldots, (n+m+p) \), \( k = (n+m+p+1), \ldots, (m+n+p+q) \), \( j = 1, 2, \ldots, (n+m+p+q) \), respectively. The first \( m \) rows of the matrix \( A \) leads to values of measurements, the next \( n \) rows - to values of the right-hand side of the initial condition and, of course, time variable is then equal to zero, the next \( p \) rows leads to values of the right-hand side of the Dirichlet condition and the last \( q \) rows - to values of the right-hand side of Neumann condition.
The solvability of the system (31) depends on the non-singularity of the matrix $A$, which is still an open research problem.

Fundamental solution method belongs to the family of Trefftz method. Both methods, described in part 4.4 and 4.6, frequently lead to ill-conditioned system of algebraic equation. To solve the system of equations, different techniques are used. Two of them, namely single value decomposition and Tikhonov regularization technique, are briefly presented in the further parts of the chapter.

### 4.7 Singular value decomposition

The ill-conditioning of the coefficient matrix $A$ (formula (32) in the previous part of the chapter) indicates that the numerical result is sensitive to the noise of the right hand side $\tilde{b}$ (formula (33)) and the number of collocation points. In fact, the condition number of the matrix $A$ increases dramatically with respect to the total number of collocation points.

The singular value decomposition usually works well for the direct problems but usually fails to provide a stable and accurate solution to the system (31). However, a number of regularization methods have been developed for solving this kind of ill-conditioning problem, (Hansen, 1992; Hansen & O’Leary, 1993). Therefore, it seems useful to present the singular value decomposition method here.

Denote $N = n + m + p + q$. The singular value decomposition of the $N \times N$ matrix $A$ is a decomposition of the form

$$ A = W \Sigma V^T = \sum_{i=1}^{N} w_i \sigma_i v_i^T $$

with $W = (w_1, w_2, ..., w_N)$ and $V = (v_1, v_2, ..., v_N)$ satisfying $W^T W = V^T V = I_N$. Here, the superscript $T$ denotes transposition of a matrix. It is known that $\Sigma = \text{diag}(\sigma_1, \sigma_2, ..., \sigma_N)$ has non-negative diagonal elements satisfying inequality

$$ \sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_N \geq 0 $$

The values $\sigma_i$ are called the singular values of $A$ and the vectors $w_i$ and $v_i$ are called left and right singular vectors of $A$, respectively, (Golub & Van Loan, 1998). The more rapid is the decrease of singular values in (35), the less we can reconstruct reliably for a given noise level. Equivalently, in order to get good reconstruction when the singular values decrease rapidly, an extremely high signal-to-noise ratio in the data is required.

For the matrix $A$ the singular values decay rapidly to zero and the ratio between the largest and the smallest nonzero singular values is often huge. Based on the singular value decomposition, it is easy to know that the solution for the system (31) is given by

$$ \tilde{\lambda} = \sum_{i=1}^{N} \frac{w_i^T \tilde{b}}{\sigma_i} v_i $$

When there are small singular values, such approach leads to a very bad reconstruction of the vector $\tilde{\lambda}$. It is better to consider small singular values as being effectively zero, and to regard the components along such directions as being free parameters which are not determined by the data.
However, as it was stated above, the singular value decomposition usually fails for the inverse problems. Therefore it is better to use here Tikhonov regularization method.

4.8 Tikhonov regularization method

This is perhaps the most common and well known of regularization schemes, (Tikhonov & Arsenin, 1977). Instead of looking directly for a solution for an ill-posed problem (31) we consider a minimum of a functional

$$J[\hat{x}] = \| A\hat{x} - \hat{b} \|^2 + \alpha^2 \| \hat{x} - \hat{x}_0 \|^2$$

(37)

with \( \hat{x}_0 \) being a known vector, \( \| \cdot \| \) denotes the Euclidean norm, and \( \alpha^2 \) is called the regularization parameter. The necessary condition of minimum of the functional (37) leads to the following system of equation:

$$A^T (A\hat{x} - \hat{b}) + \alpha^2 (\hat{x} - \hat{x}_0) = 0 .$$

Hence

$$\hat{x} = \left( A^T A + \alpha^2 I \right)^{-1} \left( A^T \hat{b} + \alpha^2 \hat{x}_0 \right)$$

Taking into account (34) after transformation one obtains the following form of the functional \( J[y] \):

$$J[\hat{x}] = \| V\Sigma V^T \hat{x} - WW^T \hat{b} \|^2 + \alpha^2 \| VV^T (\hat{x} - \hat{x}_0) \|^2$$

$$= \| V(\Sigma y - c) \|^2 + \alpha^2 \| V(y - y_0) \|^2 = \| \Sigma y - c \|^2 + \alpha^2 \| y - y_0 \|^2 = J[y]$$

(38)

where \( y = V^T \hat{x} \), \( y_0 = V^T \hat{x}_0 \), \( c = W^T \hat{b} \) and the use has been made from the properties \( W^T W = V^T V = I_N \). Minimization of the functional \( J[y] \) leads to the following vector equation:

$$\Sigma^T (\Sigma y - c) + \alpha^2 (y - y_0) = 0 \quad \text{or} \quad (\Sigma^T \Sigma + \alpha^2) y = \Sigma^T c + \alpha^2 y_0 .$$

Hence

$$y_i = \frac{\sigma_i}{\sigma_i^2 + \alpha^2} c_i + \frac{\alpha^2}{\sigma_i^2 + \alpha^2} y_{0i} , \quad i = 1, \ldots, N \quad \text{or} \quad \hat{x} = \sum_{i=1}^{N} \left( \frac{\sigma_i}{\sigma_i^2 + \alpha^2} W_i^T b_i + \frac{\alpha^2}{\sigma_i^2 + \alpha^2} \hat{x}_0 \right)$$

(39)

If \( \hat{x}_0 = 0 \) the Tikhonov regularized solution for equation (31) based on singular value decomposition of the \( N \times N \) matrix \( A \) can be expressed as

$$\hat{x}_N = \sum_{i=1}^{N} \frac{\sigma_i}{\sigma_i^2 + \alpha^2} W_i^T b_i$$

(40)
The determination of a suitable value of the regularization parameter $\alpha^2$ is crucial and is still under intensive research. Recently the L-curve criterion is frequently used to choose a good regularization parameter, (Hansen, 1992; Hansen & O’Leary, 1993). Define a curve $L$ by

$$L = \left[ \log \left( \frac{\|A\tilde{u}\|}{\|\tilde{u}\|} \right), \log \left( \frac{\|A\tilde{u} - \delta\|}{\|\delta\|} \right) \right]$$

(41)

A suitable regularization parameter $\alpha^2$ is the one near the “corner” of the L-curve, (Hansen & O’Leary, 1993; Hansen, 2000).

4.9 The conjugate gradient method

The conjugate gradient method is a straightforward and powerful iterative technique for solving linear and nonlinear inverse problems of parameter estimation. In the iterative procedure, at each iteration a suitable step size is taken along a direction of descent in order to minimize the objective function. The direction of descent is obtained as a linear combination of the negative gradient direction at the current iteration with the direction of descent of the previous iteration. The linear combination is such that the resulting angle between the direction of descent and the negative gradient direction is less than $90^\circ$ and the minimization of the objective function is assured, (Özisik & Orlande, 2000).

As an example consider the following problem in a flat slab with the unknown heat source $g_p(t)$ in the middle plane:

$$\frac{\partial^2 T}{\partial x^2} + g_p(t)\delta(x - 0.5) = \frac{\partial T}{\partial t} \quad \text{in} \quad 0 < x < 1, \text{for} \ t > 0$$

$$\frac{\partial T}{\partial x} = 0 \quad \text{at} \ x = 0 \quad \text{and} \ x = 1, \text{for} \ t > 0$$

$$T(x,0) = 0 \quad \text{for} \ t = 0, \text{in} \ 0 < x < 1$$

(42)

where $\delta(\cdot)$ is the Dirac delta function. Application of the conjugate gradient method can be organized in the following steps (Özisik & Orlande, 2000):

- The direct problem,
- The inverse problem,
- The iterative procedure,
- The stopping criterion,
- The computational algorithm.

The direct problem. In the direct problem associated with the problem (42) the source strength, $g_p(t)$, is known. Solving the direct problem one determines the transient temperature field $T(x,t)$ in the slab.

The inverse problem. For solution of the inverse problem we consider the unknown energy generation function $g_p(t)$ to be parameterized in the following form of linear combination of trial functions $C_j(t)$ (e.g. polynomials, B-splines, etc.):
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\[ S_p(t) = \sum_{j=1}^{N} p_j C_j(t) \]  \hspace{1cm} (43)

\( p_j \) are unknown parameters, \( j = 1,2,...,N \). The total number of parameters, \( N \), is specified. The solution of the inverse problem is based on minimization of the ordinary least square norm, \( S(P) \):

\[ S(P) = \sum_{i=1}^{I} [Y_i - T_i(P)]^2 = [Y - T(P)]^T [Y - T(P)] \]  \hspace{1cm} (44)

where \( P^T = [p_1,p_2,...,p_N] \), \( T_i(P) = T(P,t_i) \) states for estimated temperature at time \( t_i \), \( Y_i = Y(t_i) \) denotes measured temperature at time \( t_i \), \( I \) is a total number of measurements, \( I \geq N \). The parameters estimation problem is solved by minimization of the norm (44).

**The iterative procedure.** The iterative procedure for the minimization of the norm \( S(P) \) is given by

\[ P^{k+1} = P^k - \beta^k d^k \]  \hspace{1cm} (45)

where \( \beta^k \) is the search step size, \( d^k = [d_1^k,d_2^k,...,d_N^k] \) is the direction of descent and \( k \) is the number of iteration. \( d^k \) is a conjugation of the gradient direction, \( \nabla S(P^k) \), and the direction of descent of the previous iteration, \( d^{k-1} \):

\[ d^k = \nabla S(P^k) + \gamma^k d^{k-1} \]  \hspace{1cm} (46)

Different expressions are available for the conjugation coefficient \( \gamma^k \). For instance the Fletcher-Reeves expression is given as

\[ \gamma^k = \frac{\sum_{j=1}^{N} [\nabla S(P^k)]_j^2}{\sum_{j=1}^{N} [\nabla S(P^{k-1})]_j^2} \]  \hspace{1cm} (47)

Here

\[ [\nabla S(P^k)]_j = -2 \sum_{i=1}^{I} \frac{\partial T_i}{\partial P_j} [Y_i - T_i(P^k)] \]  \hspace{1cm} (48)

Note that if \( \gamma^k = 0 \) for all iterations \( k \), the direction of descent becomes the gradient direction in (46) and the steepest-descent method is obtained.

The search step \( \beta^k \) is obtained by minimizing the function \( S(P^{k+1}) \) with respect to \( \beta^k \). It yields the following expression for \( \beta^k \):

\[ \beta^k = \frac{\sum_{i=1}^{I} (Y_i - T_i(P^k))^2}{\sum_{j=1}^{N} [\nabla S(P^{k-1})]_j^2} \]

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The stopping criterion. The iterative procedure does not provide the conjugate gradient method with the stabilization necessary for the minimization of $S(P)$ to be classified as well-posed. Such is the case because of the random errors inherent to the measured temperatures. However, the method may become well-posed if the Discrepancy Principle is used to stop the iterative procedure, (Alifanov, 1994):

$$S(P^{k+1}) < \varepsilon$$

(50)

where the value of the tolerance $\varepsilon$ is chosen so that sufficiently stable solutions are obtained, i.e. when the residuals between measured and estimated temperatures are of the same order of magnitude of measurement errors, that is $|\hat{Y}(t_i) - T(x_{\text{meas}}, t_i)| \approx \sigma_i$, where $\sigma_i$ is the standard deviation of the measurement error at time $t_i$. For $\sigma_i = \sigma = \text{const}$ we obtain $\varepsilon = I\sigma$. Such a procedure gives the conjugate gradient method an iterative regularization character. If the measurements are regarded as errorless, the tolerance $\varepsilon$ can be chosen as a sufficiently small number, since the expected minimum value for the $S(P)$ is zero.

The computation algorithm. Suppose that temperature measurements $Y = [Y_1, Y_2, ..., Y_I]$ are given at times $t_i$, $i = 1, 2, ..., I$, and an initial guess $P^0$ is available for the vector of unknown parameters $P$. Set $k = 0$ and then

Step 1. Solve the direct heat transfer problem (42) by using the available estimate $P^k$ and obtain the vector of estimated temperatures $T(P^k) = [T_1, T_2, ..., T_I]$.

Step 2. Check the stopping criterion given by equation (50). Continue if not satisfied.

Step 3. Compute the gradient direction $\nabla S(P^k)$ from equation (48) and then the conjugation coefficient $\gamma^k$ from (47).

Step 4. Compute the direction of descent $d^k$ by using equation (46).

Step 5. Compute the search step size $\beta^k$ from formula (49).

Step 6. Compute the new estimate $P^{k+1}$ using (45).

Step 7. Replace $k$ by $k+1$ and return to step 1.

4.10 The Levenberg-Marquardt method

The Levenberg-Marquardt method, originally devised for application to nonlinear parameter estimation problems, has also been successfully applied to the solution of linear ill-conditioned problems. Application of the method can be organized as for conjugate gradient. As an example we will again consider the problem (42).

The first two steps, the direct problem and the inverse problem, are the same as for the conjugate gradient method.
The iterative procedure. To minimize the least squares norm, (44), we need to equate to zero the derivatives of \( S(P) \) with respect to each of the unknown parameters \( [P_1, P_2, ..., P_N] \), that is,

\[
\frac{\partial S(P)}{\partial P_1} = \frac{\partial S(P)}{\partial P_2} = ... = \frac{\partial S(P)}{\partial P_N} = 0
\]  

(51)

Let us introduce the Sensitivity or Jacobian matrix, as follows:

\[
J(P) = \left[ \frac{\partial T_j}{\partial P_i} \right]_{i,j=1}^{N} = \left[ \frac{\partial T_j}{\partial P_i} \right]_{i,j=1}^{N}
\]

(52)

where \( N = \) total number of unknown parameters, \( I = \) total number of measurements. The elements of the sensitivity matrix are called the sensitivity coefficients, (Özisik & Orlande, 2000). The results of differentiation (51) can be written down as follows:

\[
-2J^T(P)[Y - T(P)] = 0
\]

(53)

For linear inverse problem the sensitivity matrix is not a function of the unknown parameters. The equation (53) can be solved then in explicit form (Beck & Arnold, 1977):

\[
P = (J^T J)^{-1} J^T Y
\]

(54)

In the case of a nonlinear inverse problem, the matrix \( J \) has some functional dependence on the vector \( P \). The solution of equation (53) requires then an iterative procedure, which is obtained by linearizing the vector \( T(P) \) with a Taylor series expansion around the current solution at iteration \( k \). Such a linearization is given by

\[
T(P) = T(P^k) + J^k (P - P^k)
\]

(55)

where \( T(P^k) \) and \( J^k \) are the estimated temperatures and the sensitivity matrix evaluated at iteration \( k \), respectively. Equation (55) is substituted into (54) and the resulting expression is rearranged to yield the following iterative procedure to obtain the vector of unknown parameters \( P \) (Beck & Arnold, 1977):

\[
P^{k+1} = P^k + [(J^k)^T J^k]^{-1} (J^k)^T [Y - T(P^k)]
\]

(56)

The iterative procedure given by equation (56) is called the Gauss method. Such method is actually an approximation for the Newton (or Newton-Raphson) method. We note that
equation (54), as well as the implementation of the iterative procedure given by equation (56), require the matrix $J^T J$ to be nonsingular, or

$$|J^T J| \neq 0 \quad (57)$$

where $|.|$ is the determinant.

Formula (57) gives the so called Identifiability Condition, that is, if the determinant of $J^T J$ is zero, or even very small, the parameters $p_j$, for $j = 1,2,...,N$, cannot be determined by using the iterative procedure of equation (56).

Problems satisfying $|J^T J| = 0$ are denoted ill-conditioned. Inverse heat transfer problems are generally very ill-conditioned, especially near the initial guess used for the unknown parameters, creating difficulties in the application of equations (54) or (56). The Levenberg-Marquardt method alleviates such difficulties by utilizing an iterative procedure in the form, (Özisik & Orlande, 2000):

$$P^{k+1} = P^k + (J^T J^k + \mu^k \Omega^k)^{-1} (J^T k^k Y - T(P^k)) \quad (58)$$

where $\mu^k$ is a positive scalar named damping parameter and $\Omega^k$ is a diagonal matrix.

The purpose of the matrix term $\mu^k \Omega^k$ is to damp oscillations and instabilities due to the ill-conditioned character of the problem, by making its components large as compared to those of $J^T J$ if necessary. $\mu^k$ is made large in the beginning of the iterations, since the problem is generally ill-conditioned in the region around the initial guess used for iterative procedure, which can be quite far from the exact parameters. With such an approach, the matrix $J^T J$ is not required to be non-singular in the beginning of iterations and the Levenberg-Marquardt method tends to the steepest descent method, that is, a very small step is taken in the negative gradient direction. The parameter $\mu^k$ is then gradually reduced as the iteration procedure advances to the solution of the parameter estimation problem, and then the Levenberg-Marquardt method tends to the Gauss method given by (56).

The stopping criteria. The following criteria were suggested in (Dennis & Schnabel, 1983) to stop the iterative procedure of the Levenberg-Marquardt Method given by equation (58):

$$S[P^{k+1}] < \epsilon_1$$

$$\|J^k (Y - T(P^k))\| < \epsilon_2$$

$$\|P^{k+1} - P^k\| < \epsilon_3 \quad (59)$$

where $\epsilon_1$, $\epsilon_2$ and $\epsilon_3$ are user prescribed tolerances and $\|\|$ denotes the Euclidean norm.

The computational algorithm. Different versions of the Levenberg-Marquardt method can be found in the literature, depending on the choice of the diagonal matrix $d$ and on the form chosen for the variation of the damping parameter $\mu^k$ (Özisik & Orlande, 2000), [I-91. Here
\[ \Omega^k = \text{diag}([J^k]^T J^k) . \] 

Suppose that temperature measurements \( Y = [Y_1, Y_2, \ldots, Y_I] \) are given at times \( t_i \), \( i = 1, 2, \ldots, I \), and an initial guess \( P^0 \) is available for the vector of unknown parameters \( P \). Choose a value for \( \mu^0 \), say, \( \mu^0 = 0.001 \) and set \( k=0 \). Then,

1. Solve the direct heat transfer problem (42) with the available estimate \( P^k \) in order to obtain the vector \( T(P^k) = [T_1, T_2, \ldots, T_I] \).

2. Compute \( S(P^k) \) from the equation (44).

3. Compute the sensitivity matrix \( J^k \) from (52) and then the matrix \( \Omega^k \) from (60), by using the current value of \( P^k \).

4. Solve the following linear system of algebraic equations, obtained from (58):

\[ [(J^k)^T J^k + \mu^k \Omega^k] \Delta P^k = (J^k)^T [Y - T(P^k)] \] 

in order to compute \( \Delta P^k = P^{k+1} - P^k \).

5. Compute the new estimate \( P^{k+1} \) as

\[ P^{k+1} = P^k + \Delta P^k \] 

6. Solve the exact problem (42) with the new estimate \( P^{k+1} \) in order to find \( T(P^{k+1}) \).

Then compute \( S(P^{k+1}) \).

7. If \( S(P^{k+1}) \geq S(P^k) \), replace \( \mu^k \) by \( 10 \mu^k \) and return to step 4.

8. If \( S(P^{k+1}) \leq S(P^k) \), accept the new estimate \( P^{k+1} \) and replace \( \mu^k \) by \( 0.1 \mu^k \).

9. Check the stopping criteria given by (59). Stop the iterative procedure if any of them is satisfied; otherwise, replace \( k \) by \( k+1 \) and return to step 3.

### 4.11 Kalman filter method

Inverse problems can be regarded as a case of system identification problems. System identification has enjoyed outstanding attention as a research subject. Among a variety of methods successfully applied to them, the Kalman filter, (Kalman, 1960; Norton, 1986; Kurpisz & Nowak, 1995), is particularly suitable for inverse problems.

The Kalman filter is a set of mathematical equations that provides an efficient computational (recursive) solution of the least-squares method. The Kalman filtering technique has been chosen extensively as a tool to solve the parameter estimation problem. The technique is simple and efficient, takes explicit measurement uncertainty incrementally (recursively), and can also take into account a priori information, if any.

The Kalman filter estimates a process by using a form of feedback control. To be precise, it estimates the process state at some time and then obtains feedback in the form of noisy measurements. As such, the equations for the Kalman filter fall into two categories: time update and measurement update equations. The time update equations project forward (in time) the current state and error covariance estimates to obtain the a priori estimates for the next time step. The measurement update equations are responsible for the feedback by
incorporating a new measurement into the \textit{a priori} estimate to obtain an improved \textit{a posteriori} estimate. The time update equations are thus predictor equations while the measurement update equations are corrector equations.

The standard Kalman filter addresses the general problem of trying to estimate $x \in \mathbb{R}$ of a dynamic system governed by a linear stochastic difference equation, (Neaupane \\& Sugimoto, 2003)

### 4.12 Finite element method

The finite element method (FEM) or finite element analysis (FEA) is based on the idea of dividing the complicated object into small and manageable pieces. For example a two-dimensional domain can be divided and approximated by a set of triangles or rectangles (the elements or cells). On each element the function is approximated by a characteristic form.

The theory of FEM is well known and described in many monographs, e.g. (Zienkiewicz, 1977; Reddy \\& Gartling, 2001). The classic FEM ensures continuity of an approximate solution on the neighbouring elements. The solution in an element is built in the form of linear combination of shape function. The shape functions in general do not satisfy the differential equation which describes the considered problem. Therefore, when used to solve approximately an inverse heat transfer problem, usually leads to not satisfactory results.

The FEM leads to promising results when T-functions (see part 4.4) are used as shape functions. Application of the T-functions as base functions of FEM to solving the inverse heat conduction problem was reported in (Ciałkowski, 2001). A functional leading to the Finite Element Method with Trefftz functions may have other interpretation than usually accepted. Usually the functional describes mean-square fitting of the approximated temperature field to the initial and boundary conditions. For heat conduction equation the functional is interpreted as mean-square sum of defects in heat flux flowing from element to element, with condition of continuity of temperature in the common nodes of elements. Full continuity between elements is not ensured because of finite number of base functions in each element.

However, even the condition of temperature continuity in nodes may be weakened. Three different versions of the FEM with T-functions (FEMT) are considered in solving inverse heat conduction problems: (a) FEMT with the condition of continuity of temperature in the common nodes of elements, (b) no temperature continuity at any point between elements and (c) nodeless FEMT.

Let us discuss the three approaches on an example of a dimensionless 2D transient boundary inverse problem in a square $\Omega = \{(x, y): 0 < x < 1, \ 0 < y < 1\}$, for $t > 0$. Assume that for $y = 0$ the boundary condition is not known; instead measured values of temperature, $y_{ik}$, are known at points $(1 - \delta_{ik}, y_i, t_k)$. Furthermore,

\[
T(x, y, t) \big|_{t=0} = T_0(x, y), \quad T(x, y, t) \big|_{y=0} = h_1(y, t), \quad \frac{\partial T}{\partial y}(x, y, t) \bigg|_{y=1} = h_2(x, t),
\]

\[
\left. \frac{\partial T}{\partial y}(x, y, t) \right|_{y=0} = h_3(x, t)
\]

(63)
(a) FEMT with the condition of continuity of temperature in the common nodes of elements (Figure 2). We consider time-space finite elements. The approximate temperature in a \( j \)-th element, \( \hat{T}^j(x,y,t) \), is a linear combination of the T-functions, \( V_m(x,y,t) \):

\[
T^j(x,y,t) = \hat{T}^j(x,y,t) = \sum_{m=1}^{N_j} c_{mj} V_m(x,y,t) = [C]^T [V(x,y,t)]
\]  

(64)

where \( N \) is the number of nodes in the \( j \)-th element and \( [V(x, y, t)] \) is the column matrix consisting of the T-functions. The continuity of the solution in the nodes leads to the following matrix equation in the element:

\[
[VV][C] = [T]
\]  

(65)

In (65) elements of matrix \([VV]\) stand for values of the T-functions, \( V_m(x,y,t) \), in the nodal points, i.e. \( V_{rs} = V_s(x_r,y_s,t_j), \quad r,s = 1,2,...,N \). The column matrix \([T]=[T^1, T^2, ..., T^N]^T\) consists of temperatures (mostly unknown) of the nodal points with \( T^i \) standing for value of temperature in the \( i \)-th node, \( i = 1,2,...,N \). The unknown coefficients of the linear combination (63) are the elements of the column matrix \([C]\). Hence we obtain

\[
[C]=[VV]^{-1}[T] \quad \text{and finally} \quad \hat{T}^j(x,y,t) = ([VV]^{-1}[T])^T [V(x,y,t)]
\]  

(66)

It is clear, that in each element the temperature \( \hat{T}^j(x,y,t) \) satisfies the heat conduction equation. The elements of matrix \(([VV]^{-1}[T])^T\) can be calculated from minimization of the objective functional, describing the mean-square fitting of the approximated temperature field to the initial and boundary conditions.

Fig. 2. Time-space elements in the case of temperature continuous in the nodes.

(b) No temperature continuity at any point between elements (Figure 3). The approximate temperature in a \( j \)-th element, \( \hat{T}^j(x,y,t) \), is a linear combination of the T-functions (63), too. In this case in order to ensure the physical sense of the solution we minimize inaccuracy of the temperature on the borders between elements. It means that the functional describing the mean-square fitting of the approximated temperature field to
the initial and boundary conditions includes the temperature jump on the borders between elements. For the case

\[
J = \sum_{i} \left( \int_{\Omega_i} \left( \tilde{T}_i(x,y,0) - T_0(x,y) \right)^2 \, d\Omega + \int_{\Gamma_i} \left( \tilde{T}_i(0,y,t) - h_1(y,t) \right)^2 \, d\Gamma \right) + \sum_{k} \int_{\Omega_k} \left( \frac{\partial \tilde{T}_k(x,t)}{\partial y} - h_2(x,t) \right)^2 \, d\Omega + \sum_{k} \int_{\Gamma_k} \left( \frac{\partial \tilde{T}_k(x,0,t)}{\partial y} - h_3(x,t) \right)^2 \, d\Gamma
\]

\[
+ \sum_{i,j} \int_{\Gamma_{i,j}} \left( \tilde{T}_i - \tilde{T}_j \right)^2 \, d\Gamma + \sum_{k=1}^{m} \sum_{i=1}^{k} \left( \tilde{T}_i(x_i,y_i,t) - Y_{ik} \right)^2 \right|_{t=k-1,t_k}
\]

(67)

Fig. 3. Time-space elements in the case of temperature discontinuous in the nodes.

(c) Nodeless FEMT. Again, \( \tilde{T}_i(x,y,t) \) is a linear combination of the T-functions. The time interval is divided into subintervals. In each subinterval the domain \( \Omega \) is divided into \( J \) subdomains (finite elements) and in each subdomain \( \Omega_j, j=1, 2, \ldots, J \) (with \( \Gamma_i = \partial \Omega_i \)) the temperature is approximated with the linear combination of the Trefftz functions according to the formula (64). The dimensionless time belongs to the considered subinterval. In the case of the first subinterval an initial condition is known. For the next subintervals initial condition is understood as the temperature distribution in the subdomain \( \Omega_j \) at the final moment of time in the previous subinterval. The mean-square method is used to minimize the inaccuracy of the approximate solution on the boundary, at the initial moment of time and on the borders between elements. This way the unknown coefficients of the combination, \( c_{ij}^m \), can be calculated. Generally, the coefficients \( c_{ij}^m \) depend on the time subinterval number, (Grysa & Lesniewska, 2009).

In (Ciałkowski et al., 2007) the FEM with Trefftz base functions (FEMT) has been compared with the classic FEM approach. The FEM solution of the inverse problem for the square considered was analysed. For the FEM the elements with four nodes and, consequently, the simplest set of base functions: \( (1, x, y, xy) \) have been applied.

Consider an inverse problem in a square (compare the paragraph before the equation (63)). Using FEM to solve the inverse problem gives acceptable solution only for the first row of elements. Even for exact values of the given temperature the results are encumbered with
relatively high error. For the next row of the elements, the FEM solution is entirely not acceptable. When the distance $\delta_y$ greater than the size of the element, an instability of the numerical solution appears independently of the number of finite elements. Paradoxically, the greater number of elements, the sooner the instability appears even though the accuracy of solution in the first row of elements becomes better. The classic FEM leads to much worse results than the FEMT because the latter makes use of the Trefftz functions which satisfy the energy equation. This way the physical meaning of the results is ensured.

4.13 Energetic regularization in FEM

Three kinds of physical aspects of heat conduction can be applied to regularize an approximate solution obtained with the use of finite element method, (Ciałkowski et al., 2007). The first is minimization of heat flux jump between the elements, the second is minimization of the defect of energy dissipation on the border between elements and the third is the minimization of the intensity of entropy production between elements. Three kinds of regularizing terms for the objective functional are proposed:

- minimizing the heat flux inaccuracy between elements:

  \[
  \sum_{i,j}^{t_f} dt \int_{\Gamma_{ij}} \left( \frac{\partial T_i}{\partial n_i} - \frac{\partial T_j}{\partial n_j} \right)^2 d\Gamma \tag{68}
  \]

- minimizing numerical entropy production between elements:

  \[
  \sum_{i,j}^{t_f} dt \int_{\Gamma_{ij}} \left( 1 - \frac{\partial T_i}{\partial T_j} \right)^2 d\Gamma , \text{ and} \tag{69}
  \]

- minimizing the defect of energy of dissipation between elements:

  \[
  \sum_{i,j}^{t_f} dt \int_{\Gamma_{ij}} \left( \frac{\partial T_i}{\partial n_i} \ln T_i - \frac{\partial T_j}{\partial n_j} \ln T_j \right)^2 d\Gamma \tag{70}
  \]

with $t_f$ being the final moment of the considered time interval, (Ciałkowski et al., 2007; Grysa & Leśniewska, 2009), and $\Gamma_{ij}$ standing for the border between $i$-th and $j$-th element.

Notice that entropy production functional and energy dissipation functional are not quadratic functions of the coefficients of the base functions in elements. Hence, minimizing the objective functional leads to a non-linear system of algebraic equations. It seems to be the only disadvantage when compared with minimizing mean-square defects of heat flux (formula (68)); the latter leads to a system of linear equations.

4.14 Other methods

Many other methods are used to solve the inverse heat conduction problems. Many iterative methods for approximate solution of inverse problems are presented in monograph (Bakushinsky & Kokurin, 2004). Numerical methods for solving inverse problems of mathematical physics are presented in monograph (Samarski & Vabishchevich, 2007). Among other methods it is worth to mention boundary element method (Bialecki et al., 2006; Onyango...
et al., 2008), the finite difference method (Luo & Shih, 2005; Soti et al., 2007), the theory of potentials method (Grysa, 1989), the radial basis functions method (Kołodziej et al., 2010), the artificial bee colony method (Hetmaniok et al., 2010), the Alifanov iterative regularization (Alifanov, 1994), the optimal dynamic filtration, (Guzik & Styrylska, 2002), the control volume approach (Taler & Zima, 1999), the meshless methods (Sladek et al., 2006) and many other.

5. Examples of the inverse heat conduction problems

5.1 Inverse problems for the cooled gas turbine blade

Let us consider the following stationary problem concerning the gas turbine blade (Figure 4): find temperature distribution on the inner boundary \( \Gamma \) of the blade cross-section, \( T_{\Gamma} \), and heat transfer coefficient variation along \( \Gamma \), with the condition

\[
T_0 - \epsilon_T \leq T(s) \leq T_0 + \epsilon_T
\]

(71)

where \( \epsilon_T \) stands for temperature measurement tolerance and \( s \) is a normalized coordinate of a perimeter length (black dots in Figure 4 denote the beginning and the end of the inner and outer perimeter, coordinate is counted counterclockwise). Heat transfer coefficient distribution at the outer surface, \( h_{\Gamma} \), is known, \( T_{fo} = 1350^\circ C, T_{fi} = 780^\circ C, T_0 = 1100^\circ C, \epsilon_T \), standing for temperature measurement tolerance, does not exceed \( 1^\circ C \). Moreover, the inner and outer fluid temperature \( T_{fo} \) and \( T_{fi} \) are known, (Ciałkowski et al., 2007a). The unknowns: \( T_{\Gamma} \), \( h_{\Gamma} \). The solution has to be found in the class of functions fulfilling the energy equation

\[
\nabla (k \nabla T) = 0
\]

(72)

with \( k \) assumed to be a constant. To solve the problem we use FEM with the shape functions belonging to the class of harmonic functions. It means that we can express an approximate
solution of a stationary heat conduction problem in each element as a linear combination of the T-functions suitable for the equation (72). The functional with a term minimizing the heat flux inaccuracy between elements reads

$$I_q(T) = \sum \left[ \int_{\Gamma_{ij}} (q_i - q_j)^2 d\Gamma + w \int_{\Gamma_{ij}} (T_i - T_j)^2 d\Gamma \right]$$

with

$$q = k \frac{\partial T}{\partial n}$$  \hspace{1cm} (73)

In order to simplify the problem, temperature on the outer and inner surfaces was then approximated with 5 and 30 Bernstein polynomials, respectively, in order to simplify the problem. The area of the blade cross-section was divided into 99 rectangular finite elements with 16 nodes (12 on the boundary of each element and 4 inside). 16 harmonic (Trefftz) functions were used as base functions. All together 4x297 unknowns were introduced. Calculations were carried out with the use of PC with 1.6 GHz processor. Time of calculation was 1.5 hours using authors' own computer program in Fortran F90. The results are presented at Figures 5 and 6.

![Fig. 5. Temperature [°C] (upper) and heat flux (lower) distribution on the outer (red squares) and inner (dark blue dots) surfaces of the blade.](https://www.intechopen.com)
Oscillations of temperature of the inner blade surface (Figure 5 left) is due to the number of Bernstein polynomials: it was too small. However, thanks to a small number of the polynomials a small number of unknown values of temperature could be taken for calculation. The same phenomenon appears in Figure 5 right for heat flux on the inner blade surface as well as in Figure 6 for the heat transfer coefficients values. The distance between peaks of the curves for the inner and outer surfaces in Figure 6 is a result of coordinate normalization of the inner and outer surfaces perimeter length. The normalization was done in such a way that only for \( s = 0 \) \((s = 1)\) points on both surfaces correspond to each other. The other points with the same value of the coordinate \( s \) for the outer and inner surface generally do not correspond to each other (in the case of peaks the difference is about 0.02).

Fig. 6. Heat transfer coefficient over inner (dark blue squares) and outer (red dots — given; brown dots — calculated) surfaces of the blade.

### 5.2 Direct solution of a heat transfer coefficient identification problem

Consider a 1D dimensionless problem of heat conduction in a thermally isotropic flat slab (Grysa, 1982):

\[
\frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial t} \quad \text{for} \, x \in (0, 1) \, \text{and} \, t \in (0, t_f],
\]
\[
\frac{\partial T}{\partial x} = 0 \quad \text{for } x = 0 \text{ and } t \in (0, t_f],
\]
(74)

\[
k \frac{\partial T}{\partial x} = -Bi\left[T(1,t) - T_f(t)\right] \quad \text{for } x = 1 \text{ and } t \in (0, t_f],
\]

\[T = 0 \quad \text{for } x \in (0, 1) \text{ and } t = 0.
\]

If the upper surface temperature (for \(x = 1\)) cannot be measured directly then in order to find the Biot number, temperature responses at some inner points of the slab or even temperature of the lower surface \((x = 0)\) have to be known. Hence, the problem is ill-posed.

Employing the Laplace transformation to the problem (74) we obtain

\[
\tilde{T}(x,s) = \frac{Bi \cosh x \sqrt{s}}{s \sinh \sqrt{s} + Bi \cosh \sqrt{s}} \quad \text{or}
\]

\[
\tilde{T}_f(s) \frac{\cosh x \sqrt{s}}{s \cosh \sqrt{s}} = -\frac{1}{s} \tilde{T}(x,s) + \frac{1}{Bi} \tilde{T}(x,s) \frac{\sinh \sqrt{s}}{s \cosh \sqrt{s}}
\]
(75)

The equation (75) is then used to find the formula describing the Biot number, \(Bi\). Then, the inverse Laplace transformation yields:

\[
Bi = \frac{2T(x,t) \sum_{n=1}^{\infty} \exp(-\lambda_n^2 t)}{T_f(t) \left[ 1 + 2 \sum_{n=1}^{\infty} \frac{(-1)^n}{\lambda_n} \cos(x\lambda_n) \exp(-\lambda_n^2 t) - H(t) \cdot \theta(x,t) \right]}
\]
(76)

Here asterisk denotes convolution, \(H(t)\) is the Heaviside function and \(\lambda_n = \pi(2n - 1) / 2, n = 1, 2, \ldots\).

If the temperature is known on the boundary \(x = 0\) (e.g. from measurements), values of \(Bi\) (because of noisy input data having form of a function of time) can be calculated from formula (76). Of course, formula (76) is obtained with the assumption that \(Bi = \text{const.}\) Therefore, the results have to be averaged in the considered time interval.

6. Final remarks

It is not possible to present such a broad topic like inverse heat conduction problems in one short chapter. Many interesting achievements were discussed very briefly, some were omitted. Little attention was paid to stochastic methods. Also, the non-linear issues were only mentioned when discussing some methods of solving inverse problems. For lack of space only few examples could be presented.

The inverse heat conduction problems have been presented in many monographs and tutorials. Some of them are mentioned in references, e.g. (Alifanov, 1994; Bakushinsky & Kokurin, 2004; Beck & Arnold, 1977; Grysa, 2010; Kurpisz & Nowak, 1995; Özisik & Orlande, 2000; Samarski & Vabishchevich, 2007; Duda & Taler, 2006; Hohage, 2002; Bal, 2004; Tan & Fox, 2009).
7. References


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Treffitz, E. (1926), Ein Gegenstueck zum Ritz’schen Verfahren. Proceedings of the 2nd International Congress of Applied Mechanics, pp.131–137, Orell Fussli Verlag, Zurich,


The content of this book covers several up-to-date approaches in the heat conduction theory such as inverse heat conduction problems, non-linear and non-classic heat conduction equations, coupled thermal and electromagnetic or mechanical effects and numerical methods for solving heat conduction equations as well. The book is comprised of 14 chapters divided into four sections. In the first section inverse heat conduction problems are discuss. The first two chapters of the second section are devoted to construction of analytical solutions of nonlinear heat conduction problems. In the last two chapters of this section wavelike solutions are attained. The third section is devoted to combined effects of heat conduction and electromagnetic interactions in plasmas or in pyroelectric material elastic deformations and hydrodynamics. Two chapters in the last section are dedicated to numerical methods for solving heat conduction problems.

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