# Application of the Fast Automatic Differentiation Technique for Solving Inverse Coefficient Problems

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The inverse problem of determining the thermal conductivity coefficient of substance depending on the temperature is examined and investigated.

The consideration is based on the first boundary value problem for the nonstationary heat equation.

The inverse coefficient problem is reduced to a variational problem and is solved numerically using the Fast Automatic Differentiation technique.

## Formulation of the Problem

$$C(s)\frac{\partial T}{\partial t} = div_s \left( K(T) \nabla_s T \right)$$

$$s \in Q$$

$$0 \le t \le \Theta$$
  $O \subset \mathbb{R}^n$ 

$$O \subset R^n$$

$$T(s,0) = w_0(s)$$

$$s \in Q$$

$$T(s,t) = w_{\Gamma}(s,t)$$

$$s \in \Gamma$$

$$0 \le t \le \Theta$$

 $\Gamma$  - piecewise-smooth boundary of  $\ \ Q$ 

$$s = (x_1, ..., x_n)$$
 - the Cartesian coordinates of the point

T(s,t) - the temperature of the material at the point with the coordinates S at the time t

C(s) - the volumetric heat capacity of the material

- the thermal conductivity coefficient

$$W_0(s)$$
,  $W_{\Gamma}(s,t)$  - the given temperatures

## The optimal control problem :

Find the dependence K(T) on T under which the temperature field T(s,t), obtained by solving the mixed problem, is close to the field Y(s,t), obtained experimentally, and the heat flux on the boundary of the domain is close to the experimentally data  $P(s(\Gamma),t)$ 

$$\Phi(K(T)) = \int_{0}^{\Theta} \int_{\Omega} [T(s,t) - Y(s,t)]^2 \cdot \mu(s,t) \, ds \, dt +$$

$$+ \int_{0}^{\Theta} \int_{\Gamma} \beta(s(\Gamma)) \cdot \left[ \left( -K(T(s(\Gamma),t)) \cdot \frac{\partial T(s,t)}{\partial \overline{n}} \Big|_{s \in \Gamma} \right) - P(s(\Gamma),t) \right]^{2} d\Gamma dt + \varepsilon \int_{a}^{b} (K'(T))^{2} dT$$

$$\epsilon \geq 0$$
,  $\beta(s(\Gamma)) \geq 0$ ,  $\mu(s,t) \geq 0$  - are given weight parameters  $Y(s,t)$  - the given temperature field

 $P(S(\Gamma),t)$  - the given heat flux at the boundary of the domain

The optimal control problems were solved numerically.

The cost functional was minimized using the gradient methods.

## The temperature interval [a,b] is defined as the set of values of the given functions $w_0(s), \quad w_{\Gamma}(s,t)$

The interval [a,b] is partitioned by the points  $\tilde{T}_0=a,\ \tilde{T}_1,\ \tilde{T}_2,\dots,\tilde{T}_M=b$  into M parts.

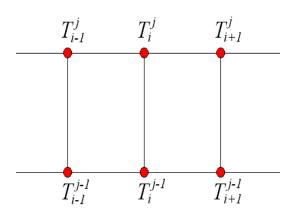
The function K(T) is approximated by a continuous piecewise linear functions with the nodes at the points  $\left\{(\widetilde{T}_m,k_m)\right\}_{m=0}^M$ 

$$K(T) = k_m + \frac{k_{m+1} - k_m}{\widetilde{T}_{m+1} - \widetilde{T}_m} (T - \widetilde{T}_m), \qquad \widetilde{T}_m \le T \le \widetilde{T}_{m+1}, \qquad k_m = K(\widetilde{T}_m)$$

Nonuniform grid: 
$$\{x_n\}_{n=0}^N$$
  $h_n^x = x_{n+1} - x_n$   $\{y_i\}_{i=0}^I$   $h_i^y = y_{i+1} - y_i$   $\{z_l\}_{l=0}^L$   $h_l^z = z_{l+1} - z_l$   $\{t^j\}_{j=0}^J$   $\tau^j = t^{j+1} - t^j$ 

A major part of the algorithm is the solution of the direct problem (determination the temperature field).

The approximation of the conjugate problem is uniquely determined by the choice of the direct problem approximation.



In one-dimensional case the direct problem is approximated by an implicit scheme with weights.

The FAD also construct an implicit scheme with weights. It is necessary to organize an iterative process to solve adjoint problem.

To approximate a direct problem in multidimensional case we propose one of variant of scheme of alternating directions.

In this case, no iterative process is required to solve the conjugate equations.

The methods of alternating directions were considered the most effective for solving three-dimensional problems of thermal conductivity:

Locally-one-dimensional schemes, the Douglas-Reckford scheme, and the Pisman-Reckford scheme

When comparing schemes, the accuracy of the resulting solution and calculation time were taken into account.

### The heat balance equation in the cell

$$\iiint_{V_{nil}} \left[ E(x, y, z, t^{j+1}) - E(x, y, z, t^{j}) \right] dV = \int_{t^{j}}^{t^{j+1}} \iint_{S_{nil}} K(T) T_{\mathbf{n}} dS dt$$

 $V_{nil}$  - the volume of the cell

 $S_{\it nil}$  - the surface of  $V_{\it nil}$ 

E(x, y, z, t)- the density of the heat content

 $T_{nil}^{\ j}$  - the average temperature in the cell at the time  $t^{\ j}$ 

 $S_{nil}^{x+}$  the part of  $S_{nil}$  that belongs to the plane  $x = \tilde{x}_{n+1}$ 

$$C_{nil} \cdot V_{nil} \cdot (T_{nil}^{j+1} - T_{nil}^{j}) \cong \int_{t^{j}}^{t^{j+1}} \left\{ \iint_{S_{nil}^{x+}} \left( K(T) \frac{\partial T}{\partial x} \right) \right|_{x = \widetilde{x}_{n+1}} dy dz - \iint_{S_{nil}^{x-}} \left( K(T) \frac{\partial T}{\partial x} \right) \right|_{x = \widetilde{x}_{n}} dy dz + C_{nil} \left( K(T) \frac{\partial T}{\partial x} \right) = C_{nil} \left( K(T) \frac{\partial$$

$$+ \iint\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{y = \tilde{y}_{n+1}} dx dz - \iint\limits_{S_{nil}^{y-}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{y = \tilde{y}_{n}} dx dz + \iint\limits_{S_{nil}^{z+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dy - \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dy - \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dy - \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dy - \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dy - \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dy - \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dy - \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dy - \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dy - \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dy - \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dy - \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dy - \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dy - \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dy - \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dy - \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dy - \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dy - \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dx dx + \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dx dx + \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dx dx + \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dx dx + \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dx dx dx + \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dx dx dx + \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dx dx dx + \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n+1}} dx dx dx dx + \int\limits_{S_{nil}^{y+}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z = \tilde{z}_{n}} \bigg|_{z = \tilde{z}_{$$

$$-\iint\limits_{S_{nil}^{z-}} \left( K(T) \frac{\partial T}{\partial x} \right) \bigg|_{z=\tilde{z}_n} dx dy dt$$

heat flux: 
$$\left(K(T)\frac{\partial T}{\partial x}\right)_{x=\tilde{x}_{n+1}} \cong \frac{K(T_{n+1,il}(t)) + K(T_{nil}(t))}{2} \cdot \frac{T_{n+1,il}(t) - T_{nil}(t)}{h_n^x}$$

#### **Notations**

$$\Lambda_{x}T_{nil}(t) = \left[\frac{K(T_{n+1,il}(t)) + K(T_{nil}(t))}{2} \cdot \frac{T_{n+1,il}(t) - T_{nil}(t)}{h_{n}^{x}} - \frac{K(T_{n,il}(t)) + K(T_{n-1,il}(t))}{2} \cdot \frac{T_{nil}(t) - T_{n-1,il}(t)}{h_{n-1}^{x}}\right] \cdot S_{il}^{yz}$$

$$\Lambda_{y}T_{nil}(t) = \left[\frac{K(T_{n,i+1,l}(t)) + K(T_{nil}(t))}{2} \cdot \frac{T_{n,i+1,l}(t) - T_{nil}(t)}{h_{i}^{y}} - \frac{T_{n,i+1,l}(t)}{h_{i}^{y}} - \frac$$

$$-\frac{K(T_{n,il}(t)) + K(T_{n,i-1,l}(t))}{2} \cdot \frac{T_{nil}(t) - T_{n,i-1,l}(t)}{h_{i-1}^{y}} \cdot S_{nl}^{xz}$$

$$\Lambda_z T_{nil}(t) = \left[ \frac{K(T_{ni,l+1}(t)) + K(T_{nil}(t))}{2} \cdot \frac{T_{ni,l+1}(t) - T_{nil}(t)}{h_l^z} - \frac{T_{nil}(t) - T_{nil}(t)}{h_l^z} \right] - \frac{1}{2} \left[ \frac{K(T_{ni,l+1}(t)) + K(T_{nil}(t))}{2} + \frac{T_{ni,l+1}(t) - T_{nil}(t)}{h_l^z} \right] - \frac{1}{2} \left[ \frac{K(T_{ni,l+1}(t)) + K(T_{nil}(t))}{2} + \frac{T_{ni,l+1}(t) - T_{nil}(t)}{h_l^z} \right] - \frac{1}{2} \left[ \frac{K(T_{ni,l+1}(t)) + K(T_{nil}(t))}{2} + \frac{T_{ni,l+1}(t) - T_{nil}(t)}{h_l^z} \right] - \frac{1}{2} \left[ \frac{K(T_{ni,l+1}(t)) + K(T_{nil}(t))}{2} + \frac{T_{ni,l+1}(t) - T_{nil}(t)}{h_l^z} \right] - \frac{1}{2} \left[ \frac{K(T_{ni,l+1}(t)) + K(T_{nil}(t))}{2} + \frac{T_{ni,l+1}(t) - T_{nil}(t)}{h_l^z} \right] - \frac{1}{2} \left[ \frac{K(T_{ni,l+1}(t)) + K(T_{nil}(t))}{2} + \frac{T_{ni,l+1}(t) - T_{nil}(t)}{h_l^z} \right] - \frac{1}{2} \left[ \frac{K(T_{ni,l+1}(t)) + K(T_{ni,l+1}(t))}{2} + \frac{T_{ni,l+1}(t) - T_{ni,l+1}(t)}{h_l^z} \right] - \frac{1}{2} \left[ \frac{K(T_{ni,l+1}(t)) + K(T_{ni,l+1}(t))}{2} + \frac{K(T_{ni,l+1}(t)) + K(T_{ni,l+1}(t))}{h_l^z} \right] - \frac{1}{2} \left[ \frac{K(T_{ni,l+1}(t)) + K(T_{ni,l+1}(t))}{2} + \frac{K(T_{ni,l+1}(t)) + K(T$$

$$-\frac{K(T_{nil}(t)) + K(T_{ni,l-1}(t))}{2} \cdot \frac{T_{nil}(t) - T_{ni,l-1}(t)}{h_{l-1}^{z}} \right] \cdot S_{ni}^{xy} \qquad S_{ni}^{xy} = \frac{h_n^x + h_{n-1}^x}{2} \cdot \frac{h_i^y + h_{i-1}^y}{2}$$

$$S_{ni}^{xy} = \frac{h_n^x + h_{n-1}^x}{2} \cdot \frac{h_i^y + h_{i-1}^y}{2}$$

$$\Lambda_{y}^{p}T_{nil}$$

$$C_{nil} \cdot V_{nil} \cdot (T_{nil}^{j+1} - T_{nil}^{j}) = \int_{t^{j}}^{t^{j+1}} \left[ \Lambda_{x} T_{nil}(t) + \Lambda_{y} T_{nil}(t) + \Lambda_{z} T_{nil}(t) \right] dt$$

$$T_{nil}^{j} \qquad T_{nil}^{j+\frac{1}{3}} \qquad T_{nil}^{j+\frac{2}{3}} \qquad t^{j} + 2\tau^{j}/3 \qquad t^{j} + 2\tau^{j}/3$$

To simplify the notation for the difference schemes, we introduce

$$\Lambda_{x}^{p}(T_{nil}^{j}) = \left[\frac{K(T_{n+1,il}^{p}) + K(T_{nil}^{p})}{2} \cdot \frac{T_{n+1,il}^{j} - T_{nil}^{j}}{h_{n}^{x}} - \frac{K(T_{nil}^{p}) + K(T_{n-1,il}^{p})}{2} \cdot \frac{T_{nil}^{j} - T_{n-1,il}^{j}}{h_{n-1}^{x}}\right] \cdot S_{il}^{yz}$$

Similar notations are introduced in the directions *x* and *y*.

When comparing schemes, the accuracy of the resulting solution and calculation time were taken into account.

## The local one-dimensional scheme

x - direction

$$\frac{V_{nil}C_{nil}(T_{nil}^{j+\frac{1}{3}}-T_{nil}^{j})}{\tau^{j}/3}=\Lambda_{x}^{p}(T_{nil}^{j+\frac{1}{3}})$$

y - direction

$$\frac{V_{nil}C_{nil}(T_{nil}^{j+\frac{2}{3}}-T_{nil}^{j+\frac{1}{3}})}{\tau^{j}/3} = \Lambda_{y}^{q}(T_{nil}^{j+\frac{2}{3}})$$

z - direction

$$\frac{V_{nil}C_{nil}(T_{nil}^{j+1}-T_{nil}^{j+\frac{2}{3}})}{\tau^{j}/3} = \Lambda_{z}^{r}(T_{nil}^{j+1})$$

$$(n=\overline{1,N-1}, \quad i=\overline{1,I-1}, \quad l=\overline{1,L-1}, \quad j=\overline{0,J-1})$$

1) 
$$p = j + 1/3$$
,  $q = j + 2/3$ ,  $r = j + 1$ 

2) 
$$p = j$$
,  $q = j + 1/3$ ,  $r = j + 2/3$ 

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## The Douglas-Reckford scheme

x - direction

$$\frac{V_{nil}C_{nil}(T_{nil}^{j+\frac{1}{3}}-T_{nil}^{j})}{\tau^{j}} = \Lambda_{x}^{j+\frac{1}{3}}(T_{nil}^{j+\frac{1}{3}}) + \Lambda_{y}^{j}(T_{nil}^{j}) + \Lambda_{z}^{j}(T_{nil}^{j})$$

y - direction

$$\frac{V_{nil}C_{nil}(T_{nil}^{j+\frac{2}{3}}-T_{nil}^{j+\frac{1}{3}})}{\tau^{j}} = \Lambda_{y}^{j+\frac{2}{3}}(T_{nil}^{j+\frac{2}{3}}) - \Lambda_{y}^{j}(T_{nil}^{j})$$

z - direction

$$\frac{V_{nil}C_{nil}(T_{nil}^{j+1}-T_{nil}^{j+\frac{2}{3}})}{\tau^{j}} = \Lambda_{z}^{j+1}(T_{nil}^{j+1}) - \Lambda_{z}^{j}(T_{nil}^{j})$$

$$(n = \overline{1, N-1}, i = \overline{1, I-1}, l = \overline{1, L-1}, j = \overline{0, J-1})$$

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## The Pisman-Reckford scheme

x - direction

$$\frac{V_{nil}C_{nil}(T_{nil}^{j+\frac{1}{3}}-T_{nil}^{j})}{\tau^{j}/3} = \Lambda_{x}^{j}(T_{nil}^{j+\frac{1}{3}}) + \Lambda_{y}^{j}(T_{nil}^{j}) + \Lambda_{z}^{j}(T_{nil}^{j})$$

y - direction

$$\frac{V_{nil}C_{nil}(T_{nil}^{j+\frac{2}{3}}-T_{nil}^{j+\frac{1}{3}})}{\tau^{j}/3} = \Lambda_{x}^{j}(T_{nil}^{j+\frac{1}{3}}) + \Lambda_{y}^{j}(T_{nil}^{j+\frac{2}{3}}) + \Lambda_{z}^{j}(T_{nil}^{j+\frac{1}{3}})$$

z - direction

$$\frac{V_{nil}C_{nil}(T_{nil}^{j+1}-T_{nil}^{j+\frac{2}{3}})}{\tau^{j}/3} = \Lambda_{x}^{j}(T_{nil}^{j+\frac{2}{3}}) + \Lambda_{y}^{j}(T_{nil}^{j+\frac{2}{3}}) + \Lambda_{z}^{j}(T_{nil}^{j+1})$$

$$(n = \overline{1, N-1}, i = \overline{1, I-1}, l = \overline{1, L-1}, j = \overline{0, J-1})$$

### **ANALYSIS OF THE OBTAINED RESULTS**

## The eciency of a particular scheme depends strongly on the dynamics of the temperature field.

The Pisman-Reckford scheme is conditionally stable, which requires the use of a much smaller step in time than the other schemes.

It is advisable to use it in cases where calculations are performed on relatively rough spatial grids (20-50 nodes in each direction).

It is reasonable to solve the variational problem on the basis of a locally one-dimensional scheme.

#### THE GRADIENT OF FUNCTIONAL IN CONTINUOUS CASE

(One-dimensional Simple Case)

Let: 
$$a = \min \left\{ \min_{x \in [0,L]} w_0(x), \min_{t \in [0,\Theta]} w_1(t), \min_{t \in [0,\Theta]} w_2(t) \right\}$$

$$b = \max \left\{ \max_{x \in [0,L]} w_0(x), \max_{t \in [0,\Theta]} w_1(t), \max_{t \in [0,\Theta]} w_2(t) \right\}$$

$$T(x,t) \in C^2(Q) \cap C^1(\overline{Q})$$
  $E(x,t) = C(x) \cdot T(x,t)$ 

$$G = \left\{K(z): K(z) \in C^1([a,b]), \ K(z) > 0, \ z \in [a,b]\right\}$$
 - the class of the feasible control functions

### The Lagrange functional:

$$I = \Phi(K(T)) + \int_{0}^{\Theta} \int_{0}^{L} \left\{ p(x,t) \left[ \frac{\partial E(T)}{\partial t} - \frac{\partial}{\partial x} \left( K(T) \frac{\partial T(x,t)}{\partial x} \right) \right] \right\} dx dt$$

$$p(x,t) \in C^{2}(Q) \cap C^{1}(\overline{Q})$$
 - an arbitrary function

### The adjoint problem

$$E'(T(x,t))\cdot\frac{\partial p(x,t)}{\partial t}+K(T)\cdot\frac{\partial^2 p(x,t)}{\partial x^2}=2\mu(x,t)\cdot(T(x,t)-Y(x,t)),$$

$$(x,t) \in Q$$
,

$$p(x,\Theta) = 0,$$

$$(0 \le x \le L)$$
,

$$p(0,t) = +2\beta \cdot (\Psi(0,t) - P_0(t)),$$

$$(0 \le t \le \Theta)$$

$$p(L,t) = -2\beta \cdot (\Psi(L,t) - P_L(t)),$$

$$(0 \le t \le \Theta)$$

$$\Psi(x,t) = -K(T(x,t)) \cdot \frac{\partial T(x,t)}{\partial x}$$

#### THE GRADIENT OF FUNCTIONAL

$$\nabla I(K(T)) = M(T), \quad T \in [a, b]$$

$$\begin{split} &\nabla I\left(K(T)\right) = \mathbf{M}(T), \quad T \in [a,b] \\ &\mathbf{M}(\eta) = \sum_{i} \int_{\xi_{Ini}^{(i)}(\eta)}^{\xi_{Fin}^{(i)}(\eta)} \left[ \frac{\partial p\left(x_{i}(\xi,\eta),t_{i}(\xi,\eta)\right)}{\partial x_{i}} \cdot sign\left(-J_{i}(\xi,\eta)\right) \frac{\partial t_{i}(\xi,\eta)}{\partial \xi} \right] d\xi, \end{split}$$

$$J_{i}(\xi,\eta) = \begin{vmatrix} \frac{\partial x_{i}(\xi,\eta)}{\partial \xi} & \frac{\partial t_{i}(\xi,\eta)}{\partial \xi} \\ \frac{\partial x_{i}(\xi,\eta)}{\partial \eta} & \frac{\partial t_{i}(\xi,\eta)}{\partial \eta} \end{vmatrix} \qquad \begin{aligned} & \chi = x_{i}(\xi,\eta) & t = t_{i}(\xi,\eta) \\ & \chi = x_{i}(\xi,\eta) & t = t_{i}(\xi,\eta) \\ & \eta = \text{const} & \text{-the isolines of the field of temperature} \end{aligned}$$

$$Q = \bigcup_{i} Q_{i}, \qquad Q_{i} \cap Q_{j} = \emptyset, \quad i \neq j$$

$$x = x_i(\xi, \eta)$$
  $t = t_i(\xi, \eta)$ 

$$\eta = const$$
 -the isolines of the field of temperature

$$\xi = const$$
 - the lines orthogonal to 
$$\eta = const$$

$$\left(\eta_{ ext{Ini}}^{(i)},\eta_{ ext{Fin}}^{(i)}
ight)$$
 - the interval of variation of the isothrems in  $Q_i$ 

$$\begin{split} \left(\xi_{\mathit{Ini}}^{(i)}(\eta), \eta\right), \left(\xi_{\mathit{Fin}}^{(i)}(\eta), \eta\right) \text{-the coordinates of the endpoints of the isotherm} \\ \eta = const \in \left(\eta_{\mathit{Ini}}^{(i)}, \eta_{\mathit{Fin}}^{(i)}\right) \text{ contained in } Q_i \end{split}$$

Fast Automatic Differentiation
Technique gives the exact components of the functional gradient for the discrete optimal control problem

Let a continuously differentiable scalar function be given

$$W(z,u)$$
, where  $z=z(u)$ 

Let a continuously differentiable vector function  $\overline{\Phi}(z,u)$  define a mapping

$$\Phi: \mathbb{R}^n \times \mathbb{R}^r \to \mathbb{R}^n$$

$$\overline{\Phi}(z,u) = \overline{0}_n$$

 $(z \in R^n, u \in R^r, 0_n - is the n - dimensional null vector)$ 

The function  $\Omega(u) = W(z(u), u)$  is a complex function

## The calculation of complex function may be represented as some multi-step process:

$$z_{i} = F(i, Z_{i}, U_{i}), \quad 1 \le i \le n \tag{1}$$

 $Z_i$  – is the set of all components of  $z_i$ , that are on the right - hand side of (1)

 $U_i$  – is the set of all components of  $u_i$ , that are on the right - hand side of (1)

Then the gradient of a complex function  $\Omega(u) = W(z(u), u)$  with respect to independent variables u is determined by the relation

$$d\Omega/du_{i} = W_{u_{i}}(z,u) + \sum_{q \in K_{i}} F_{u_{i}}(q,Z_{q},U_{q})p_{q}$$

Multipliers  $p_i \in \mathbb{R}^n$  are determined from the following system of linear algebraic equations (discrete conjugate problem):

$$p_i = W_{z_i}(z, u) + \sum_{q \in O_i} F_{z_i}(q, Z_q, U_q) p_q$$

$$Q_i = \left\{ j : 1 \le j \le n, \quad z_i \in Z_j \right\} \qquad K_i = \left\{ j : 1 \le j \le n, \quad u_i \in U_j \right\}$$

## First variational problem

("Field" functional)

It is required to find such a dependence of the thermal conductivity coefficient on temperature at which the temperature field obtained as a result of solving the direct problem differs little from the temperature field obtained experimentally.

The cost functional:

$$(\beta(s(\Gamma)) = 0, \quad \varepsilon = 0)$$

$$\Phi(K(T)) = \int_{0}^{\Theta} \int_{O} \mu(s,t) \cdot [T(s,t) - Y(s,t)]^{2} ds dt \qquad s = (x, y, z)$$

The cost functional was approximated by a function

$$F = F(k_0, k_1, ..., k_N)$$

of the finite number of variables using the method of the rectangles:

$$\Phi(K(T)) \approx F = \tau \sum_{i=1}^{J} \sum_{l=1}^{L-1} \sum_{i=1}^{I-1} \sum_{n=1}^{N-1} \left( (T_{nil}^{j} - Y_{nil}^{j})^{2} \cdot \mu_{nil}^{j} h_{n}^{x} h_{i}^{y} h_{l}^{z} \right)$$

## THE DISCRETE DIRECT PROBLEM (canonical form)

$$T_{nil}^{j+\frac{1}{3}} = T_{nil}^{j} + a_{nil} \left( K(T_{n+1,il}^{j+\frac{1}{3}}) T_{n+1,il}^{j+\frac{1}{3}} + K(T_{nil}^{j+\frac{1}{3}}) T_{n+1,il}^{j+\frac{1}{3}} - K(T_{n+1,il}^{j+\frac{1}{3}}) T_{nil}^{j+\frac{1}{3}} - K(T_{nil}^{j+\frac{1}{3}}) T_{nil}^{j+\frac{1}{3}} \right) + \\ + b_{nil} \left( K(T_{n-1,il}^{j+\frac{1}{3}}) T_{n-1,il}^{j+\frac{1}{3}} + K(T_{nil}^{j+\frac{1}{3}}) T_{n-1,il}^{j+\frac{1}{3}} - K(T_{n-1,il}^{j+\frac{1}{3}}) T_{nil}^{j+\frac{1}{3}} - K(T_{nil}^{j+\frac{1}{3}}) T_{nil}^{j+\frac{1}{3}} \right) \equiv \Psi_{nil}^{j+\frac{1}{3}} \\ \gamma - direction$$

$$\begin{split} T_{nil}^{j+\frac{2}{3}} &= T_{nil}^{j+\frac{1}{3}} + c_{nil} \left( K(T_{n,i+1,l}^{j+\frac{2}{3}}) T_{n,i+1,l}^{j+\frac{2}{3}} + K(T_{nil}^{j+\frac{2}{3}}) T_{n,i+1,l}^{j+\frac{2}{3}} - K(T_{n,i+1,l}^{j+\frac{2}{3}}) T_{nil}^{j+\frac{2}{3}} - K(T_{nil}^{j+\frac{2}{3}}) T_{nil}^{j+\frac{2}{3}} \right) + \\ &+ d_{nil} \left( K(T_{n,i-1,l}^{j+\frac{2}{3}}) T_{n,i-1,l}^{j+\frac{2}{3}} + K(T_{nil}^{j+\frac{2}{3}}) T_{n,i-1,l}^{j+\frac{2}{3}} - K(T_{n,i-1,l}^{j+\frac{2}{3}}) T_{nil}^{j+\frac{2}{3}} - K(T_{nil}^{j+\frac{2}{3}}) T_{nil}^{j+\frac{2}{3}} \right) = \Psi_{nil}^{j+\frac{2}{3}} \end{split}$$

*z* – *direction* 

$$\begin{split} T_{nil}^{j+1} &= T_{nil}^{j+\frac{2}{3}} + e_{nil} \Big( K(T_{ni,l+1}^{j+1}) T_{ni,l+1}^{j+1} + K(T_{nil}^{j+1}) T_{ni,l+1}^{j+1} - K(T_{ni,l+1}^{j+1}) T_{nil}^{j+1} - K(T_{nil}^{j+1}) T_{nil}^{j+1} \Big) + \\ &+ f_{nil} \Big( K(T_{ni,l-1}^{j+1}) T_{ni,l-1}^{j+1} + K(T_{nil}^{j+1}) T_{ni,l-1}^{j+1} - K(T_{ni,l-1}^{j+1}) T_{nil}^{j+1} - K(T_{nil}^{j+1}) T_{nil}^{j+1} \Big) \equiv \Psi_{nil}^{j+1} \end{split}$$

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## Discrete conjugate problem

#### **Notations:**

$$\begin{split} D_{nil}^{j} &= \frac{dK(T)}{dT}(T_{ni}^{j}) = \frac{k_{m} - k_{m-1}}{\widetilde{T}_{m} - \widetilde{T}_{m-1}}, \qquad (\widetilde{T}_{m-1} \leq T < \widetilde{T}_{m}) \\ A_{nil}^{j} &= \frac{d\left(K(T_{nil}^{j})T_{nil}^{j}\right)}{dT_{nil}^{j}} = D_{nil}^{j}T_{nil}^{j} + K(T_{nil}^{j}) \end{split}$$

Initial conditions for conjugate variables: (j = J)

*z* – *direction* 

$$\begin{split} p_{nil}^{J} &= \left[ e_{nil} \left( D_{nil}^{J} T_{ni,l+1}^{J} - K(T_{ni,l+1}^{J}) - A_{nil}^{J} \right) + f_{nil} \left( D_{nil}^{J} T_{ni,l-1}^{J} - K(T_{ni,l-1}^{J}) - A_{nil}^{J} \right) \right] p_{nil}^{J} - \\ &- e_{ni,l-1} \left( D_{nil}^{J} T_{ni,l-1}^{J} - K(T_{ni,l-1}^{J}) - A_{nil}^{J} \right) p_{ni,l-1}^{J} - f_{ni,l+1} \left( D_{nil}^{J} T_{ni,l+1}^{J} - K(T_{ni,l+1}^{J}) - A_{nil}^{J} \right) p_{ni,l+1}^{J} + \frac{\partial F}{\partial T_{nil}^{J}} \\ &\qquad \qquad (n = \overline{1, N-1}, \quad i = \overline{1, I-1}, \quad l = \overline{1, L-1}) \end{split}$$

$$\begin{split} p_{nil}^{j+\frac{2}{3}} &= p_{nil}^{j+1} + \left[ c_{nil} \left( D_{nil}^{j+\frac{2}{3}} T_{n,i+1,l}^{j+\frac{2}{3}} - K(T_{n,i+1,l}^{j+\frac{2}{3}}) - A_{nil}^{j+\frac{2}{3}} \right) + d_{nil} \left( D_{nil}^{j+\frac{2}{3}} T_{n,i-1,l}^{j+\frac{2}{3}} - K(T_{n,i-1,l}^{j+\frac{2}{3}}) - A_{nil}^{j+\frac{2}{3}} \right) \right] p_{nil}^{j+\frac{2}{3}} - \\ &- c_{n,i-1,l} \left( D_{nil}^{j+\frac{2}{3}} T_{n,i-1,l}^{j+\frac{2}{3}} - K(T_{n,i-1,l}^{j+\frac{2}{3}}) - A_{nil}^{j+\frac{2}{3}} \right) p_{n,i-1,l}^{j+\frac{2}{3}} - d_{n,i+1,l} \left( D_{nil}^{j+\frac{2}{3}} T_{n,i+1,l}^{j+\frac{2}{3}} - K(T_{n,i+1,l}^{j+\frac{2}{3}}) - A_{nil}^{j+\frac{2}{3}} \right) p_{n,i+1,l}^{j+\frac{2}{3}} \\ &- (n = \overline{1, N-1}, \quad i = \overline{1, I-1}, \quad l = \overline{1, L-1}, \quad j = \overline{J-1}, 0) \end{split}$$

#### x-direction

$$p_{nil}^{j+\frac{1}{3}} = p_{nil}^{j+\frac{2}{3}} + \left[ a_{nil} \left( D_{nil}^{j+\frac{1}{3}} T_{n+1,il}^{j+\frac{1}{3}} - K(T_{n+1,il}^{j+\frac{1}{3}}) - A_{nil}^{j+\frac{1}{3}} \right) + b_{nil} \left( D_{nil}^{j+\frac{1}{3}} T_{n-1,il}^{j+\frac{1}{3}} - K(T_{n-1,il}^{j+\frac{1}{3}}) - A_{nil}^{j+\frac{1}{3}} \right) \right] p_{nil}^{j+\frac{1}{3}} - a_{nil} \left( D_{nil}^{j+\frac{1}{3}} T_{n-1,il}^{j+\frac{1}{3}} - K(T_{n-1,il}^{j+\frac{1}{3}}) - A_{nil}^{j+\frac{1}{3}} \right) p_{n-1,il}^{j+\frac{1}{3}} - b_{n+1,il} \left( D_{nil}^{j+\frac{1}{3}} T_{n+1,il}^{j+\frac{1}{3}} - K(T_{n+1,il}^{j+\frac{1}{3}}) - A_{nil}^{j+\frac{1}{3}} \right) p_{n+1,il}^{j+\frac{1}{3}} - b_{n+1,il} \left( D_{nil}^{j+\frac{1}{3}} T_{n+1,il}^{j+\frac{1}{3}} - K(T_{n+1,il}^{j+\frac{1}{3}}) - A_{nil}^{j+\frac{1}{3}} \right) p_{n+1,il}^{j+\frac{1}{3}} - b_{n+1,il} \left( D_{nil}^{j+\frac{1}{3}} T_{n+1,il}^{j+\frac{1}{3}} - K(T_{n+1,il}^{j+\frac{1}{3}}) - A_{nil}^{j+\frac{1}{3}} \right) p_{n+1,il}^{j+\frac{1}{3}} - b_{n+1,il} \left( D_{nil}^{j+\frac{1}{3}} T_{n+1,il}^{j+\frac{1}{3}} - K(T_{n+1,il}^{j+\frac{1}{3}}) - A_{nil}^{j+\frac{1}{3}} \right) p_{n+1,il}^{j+\frac{1}{3}} - b_{n+1,il} \left( D_{nil}^{j+\frac{1}{3}} T_{n+1,il}^{j+\frac{1}{3}} - K(T_{n+1,il}^{j+\frac{1}{3}}) - A_{nil}^{j+\frac{1}{3}} \right) p_{n+1,il}^{j+\frac{1}{3}} - b_{n+1,il} \left( D_{nil}^{j+\frac{1}{3}} T_{n+1,il}^{j+\frac{1}{3}} - K(T_{n+1,il}^{j+\frac{1}{3}}) - A_{nil}^{j+\frac{1}{3}} \right) p_{n+1,il}^{j+\frac{1}{3}} - b_{n+1,il} \left( D_{nil}^{j+\frac{1}{3}} T_{n+1,il}^{j+\frac{1}{3}} - K(T_{n+1,il}^{j+\frac{1}{3}}) - A_{nil}^{j+\frac{1}{3}} \right) p_{n+1,il}^{j+\frac{1}{3}} - b_{n+1,il} \left( D_{nil}^{j+\frac{1}{3}} T_{n+1,il}^{j+\frac{1}{3}} - K(T_{n+1,il}^{j+\frac{1}{3}}) - A_{nil}^{j+\frac{1}{3}} \right) p_{n+1,il}^{j+\frac{1}{3}} - b_{n+1,il} \left( D_{nil}^{j+\frac{1}{3}} T_{n+1,il}^{j+\frac{1}{3}} - K(T_{n+1,il}^{j+\frac{1}{3}}) - A_{nil}^{j+\frac{1}{3}} \right) p_{n+1,il}^{j+\frac{1}{3}} - b_{n+1,il} \left( D_{nil}^{j+\frac{1}{3}} - K(T_{n+1,il}^{j+\frac{1}{3}}) - A_{nil}^{j+\frac{1}{3}} \right) p_{n+1,il}^{j+\frac{1}{3}} - b_{n+1,il}^{j+\frac{1}{3}} - b_{n+1,il}^{j+\frac{1}{3}}$$

#### z – direction

$$\begin{split} & \mathcal{L} - aurection \\ & p_{nil}^{j} = p_{nil}^{j+\frac{1}{3}} + \left[ e_{nil} \left( D_{nil}^{j} T_{ni,l+1}^{j} - K(T_{ni,l+1}^{j}) - A_{nil}^{j} \right) + f_{nil} \left( D_{nil}^{j} T_{ni,l-1}^{j} - K(T_{ni,l-1}^{j}) - A_{nil}^{j} \right) \right] p_{nil}^{j} - \\ & - e_{ni,l-1} \left( D_{nil}^{j} T_{ni,l-1}^{j} - K(T_{ni,l-1}^{j}) - A_{nil}^{j} \right) p_{ni,l-1}^{j} - f_{ni,l+1} \left( D_{nil}^{j} T_{ni,l+1}^{j} - K(T_{ni,l+1}^{j}) - A_{nil}^{j} \right) p_{ni,l+1}^{j} + \frac{\partial F}{\partial T_{nil}^{j}} \\ & (n = \overline{1,N-1}, \quad i = \overline{1,I-1}, \quad l = \overline{1,L-1}, \quad j = \overline{J-1,1}) \end{split}$$

## Formula for calculation the gradient of the cost function

$$\frac{\partial F}{\partial k_{m}} = \sum_{g=0}^{J} \sum_{r=0}^{L} \sum_{q=0}^{I} \sum_{s=0}^{N} \left( X_{rqs}^{g} \frac{\partial K(T_{rqs}^{g})}{\partial k_{m}} \right) + \sum_{g=0}^{J-1} \sum_{r=0}^{L} \sum_{q=0}^{I} \sum_{s=0}^{N} \left( X_{rqs}^{g+\frac{1}{3}} \frac{\partial K(T_{rqs}^{g+\frac{1}{3}})}{\partial k_{m}} + X_{rqs}^{g+\frac{2}{3}} \frac{\partial K(T_{rqs}^{g+\frac{2}{3}})}{\partial k_{m}} \right)$$

$$m = \overline{0, M}$$

$$\frac{\partial K(T_{nil}^{j})}{\partial k_{m-1}} = 1 - \frac{T_{ni}^{j} - \widetilde{T}_{m-1}}{\widetilde{T}_{m} - \widetilde{T}_{m-1}}; \qquad \frac{\partial K(T_{nil}^{j})}{\partial k_{m}} = \frac{T_{ni}^{j} - \widetilde{T}_{m-1}}{\widetilde{T}_{m} - \widetilde{T}_{m-1}}; \qquad \widetilde{T}_{m-1} \leq T \leq \widetilde{T}_{m}$$

$$(m = 1, ..., M)$$

$$\begin{split} \mathbf{X}_{rqs}^{g} &== \left( e_{rqs} (T_{rq,s+1}^{g} - T_{rqs}^{g}) + f_{rqs} (T_{rq,s-1}^{g} - T_{rqs}^{g}) \right) p_{rqs}^{g} + \\ &+ e_{rq,s-1} (T_{rqs}^{g} - T_{rq,s-1}^{g}) p_{rq,s-1}^{g} + f_{rq,s+1} (T_{rqs}^{g} - T_{rq,s+1}^{g}) p_{rq,s+1}^{g} \end{split}$$

$$\begin{split} \mathbf{X}_{rqs}^{g+1/3} &= \left(a_{rqs}(T_{r+1,qs}^{g+\frac{1}{3}} - T_{rqs}^{g+\frac{1}{3}}) + b_{rqs}(T_{r-1,qs}^{g+\frac{1}{3}} - T_{rqs}^{g+\frac{1}{3}})\right)p_{rqs}^{g+\frac{1}{3}} + \\ &+ a_{r-1,qs}(T_{rqs}^{g+\frac{1}{3}} - T_{r-1,qs}^{g+\frac{1}{3}})p_{r-1,qs}^{g+\frac{1}{3}} + b_{r+1,qs}(T_{rqs}^{g+\frac{1}{3}} - T_{r+1,qs}^{g+\frac{1}{3}})p_{r+1,qs}^{g+\frac{1}{3}} \end{split}$$

$$\begin{split} \mathbf{X}_{\mathit{rqs}}^{\mathit{g+2/3}} = & \left( c_{\mathit{rqs}} (T_{\mathit{r,q+1,s}}^{\mathit{g+\frac{2}{3}}} - T_{\mathit{rqs}}^{\mathit{g+\frac{2}{3}}}) + d_{\mathit{rqs}} (T_{\mathit{r,q-1,s}}^{\mathit{g+\frac{2}{3}}} - T_{\mathit{rqs}}^{\mathit{g+\frac{2}{3}}}) \right) p_{\mathit{rqs}}^{\mathit{g+\frac{2}{3}}} + \\ & + c_{\mathit{r,q-1,s}} (T_{\mathit{rqs}}^{\mathit{g+\frac{2}{3}}} - T_{\mathit{r,q-1,s}}^{\mathit{g+\frac{2}{3}}}) p_{\mathit{r,q-1,s}}^{\mathit{g+\frac{2}{3}}} + d_{\mathit{r,q+1,s}} (T_{\mathit{rqs}}^{\mathit{g+\frac{2}{3}}} - T_{\mathit{r,q+1,s}}^{\mathit{g+\frac{2}{3}}}) p_{\mathit{r,q+1,s}}^{\mathit{g+\frac{2}{3}}} \end{split}$$

Note, that the gradient of the cost function calculated using this formula is exact for the chosen approximation of the optimal control problem.



## Second variational problem

("Flux" functional)

$$\mu(x, y, z, t) \equiv 0$$

$$\Phi(K(T)) = \int_{0}^{\Theta} \iint_{\Gamma} \beta(s(\Gamma)) \cdot \left[ \left( -K(T(s(\Gamma),t)) \cdot \frac{\partial T(s,t)}{\partial \overline{n}} \right|_{s \in \Gamma} \right) - P(s(\Gamma),t) \right]^{2} d\Gamma dt$$

Find a dependence of K(T) on temperature for which the heat fluxes on the boundary of the object obtained by solving the direct problem differ little from experimental measurements.

The cost functional was approximated by a function

$$F = F(k_0, k_1, ..., k_N)$$

of the finite number of variables using the method of the rectangles.

$$\begin{split} \Phi \big( K(T) \big) &\cong F = \sum_{j=1}^{J} \left[ \sum_{l=1}^{L-1} \sum_{i=1}^{I-1} \left( \beta_{0il} \Big( H_{0il}^{\ j} - P_{0il}^{\ j} \Big)^2 + \beta_{Nil} \Big( - H_{Nil}^{\ j} - P_{Nil}^{\ j} \Big)^2 \right) \cdot h_i^y h_l^z + \\ &+ \sum_{l=1}^{L-1} \sum_{n=1}^{N-1} \left( \beta_{n0l} \Big( H_{n0l}^{\ j} - P_{n0l}^{\ j} \Big)^2 + \beta_{nIl} \Big( - H_{nIl}^{\ j} - P_{nIl}^{\ j} \Big)^2 \right) \cdot h_n^x h_l^z + \\ &+ \sum_{n=1}^{N-1} \sum_{i=1}^{I-1} \left( \beta_{ni0} \Big( H_{ni0}^{\ j} - P_{ni0}^{\ j} \Big)^2 + \beta_{niL} \Big( - H_{niL}^{\ j} - P_{niL}^{\ j} \Big)^2 \right) h_n^x h_i^y \right] \tau \end{split}$$

Through  $H_{0il}^{j}$ ,  $-H_{Nil}^{j}$ ,  $H_{n0l}^{j}$ ,  $-H_{nIl}^{j}$ ,  $H_{ni0}^{j}$  and  $-H_{niL}^{j}$  denote the heat fluxes calculated on the faces of the parallelepiped.

For example

$$H_{0il}^{j} = \frac{K(T_{1il}^{j}) + K(T_{0il}^{j})}{2} \cdot \frac{T_{1il}^{j} - T_{0il}^{j}}{h_{0}^{x}} \qquad H_{Nil}^{j} = \frac{K(T_{Nil}^{j}) + K(T_{N-1,il}^{j})}{2} \cdot \frac{T_{Nil}^{j} - T_{N-1,il}^{j}}{h_{N-1}^{x}}$$

The discrete adjoint problem, which is automatically obtained by applying the FAD technique, coincides with that presented for first variational problem, but the formulas for computing the derivatives  $\partial F / \partial T_{ni}^{\ j}$  are calculated using other formulas.

#### For example:

$$\begin{split} \frac{\partial F}{\partial T_{nil}^{j}} &= 0 & n = \overline{2, N-2}, \quad i = \overline{2, I-2}, \quad l = \overline{2, L-2} \\ \frac{\partial F}{\partial T_{0il}^{j}} &= \widetilde{A}_{il}^{j} \cdot \left[ K'(T_{0il}^{j}) \left( T_{1il}^{j} - T_{0il}^{j} \right) - \left( K(T_{0il}^{j}) + K(T_{1il}^{j}) \right) \right] & i = \overline{1, I-1}, \quad l = \overline{1, L-1} \\ \frac{\partial F}{\partial T_{1il}^{j}} &= \widetilde{A}_{il}^{j} \cdot \left[ K'(T_{1il}^{j}) \left( T_{1il}^{j} - T_{0il}^{j} \right) + \left( K(T_{0il}^{j}) + K(T_{1il}^{j}) \right) \right] & i = \overline{2, I-1}, \quad l = \overline{2, L-1} \\ \frac{\partial F}{\partial T_{N-1,il}^{j}} &= \widetilde{B}_{il}^{j} \cdot \left[ K'(T_{N-1,il}^{j}) \left( T_{Nil}^{j} - T_{N-1,il}^{j} \right) - \left( K(T_{Nil}^{j}) + K(T_{N-1,il}^{j}) \right) \right] & i = \overline{1, I-2}, \quad l = \overline{1, L-2} \\ \frac{\partial F}{\partial T_{Nil}^{j}} &= \widetilde{B}_{il}^{j} \cdot \left[ K'(T_{Nil}^{j}) \left( T_{Nil}^{j} - T_{N-1,il}^{j} \right) + \left( K(T_{Nil}^{j}) + K(T_{N-1,il}^{j}) \right) \right] & i = \overline{1, I-1}, \quad l = \overline{1, L-1} \\ \widetilde{A}_{il}^{j} &= \frac{\beta_{0il} h_{i}^{y} h_{i}^{z} \tau}{h_{i}^{x}} \left( H_{0il}^{j} - P_{0il}^{j} \right) & \widetilde{B}_{il}^{j} &= \frac{\beta_{Nil} h_{i}^{y} h_{i}^{z} \tau}{h_{N-1}^{x}} \left( H_{Nil}^{j} + P_{Nil}^{j} \right) \end{split}$$

## Formula for calculation the gradient of the cost function

$$\begin{split} \frac{\partial F}{\partial k_{m}} &= \sum_{g=0}^{J} \sum_{r=0}^{L} \sum_{q=0}^{I} \sum_{s=0}^{N} \left( X_{rqs}^{g} \frac{\partial K(T_{rqs}^{g})}{\partial k_{m}} \right) + \sum_{g=0}^{J-1} \sum_{r=0}^{L} \sum_{q=0}^{I} \sum_{s=0}^{N} \left( X_{rqs}^{g+\frac{1}{3}} \frac{\partial K(T_{rqs}^{g+\frac{1}{3}})}{\partial k_{m}} + X_{rqs}^{g+\frac{2}{3}} \frac{\partial K(T_{rqs}^{g+\frac{2}{3}})}{\partial k_{m}} \right) + \\ &+ \sum_{j=1}^{J} \left[ \sum_{l=1}^{L-1} \sum_{i=1}^{I-1} \left( \frac{\partial F}{\partial K(T_{0il}^{j})} + \frac{\partial F}{\partial K(T_{1il}^{j})} + \frac{\partial F}{\partial K(T_{N-1,il})} + \frac{\partial F}{\partial K(T_{Nil})} \right) + \\ &+ \sum_{l=1}^{L-1} \sum_{n=1}^{N-1} \left( \frac{\partial F}{\partial K(T_{n0l}^{j})} + \frac{\partial F}{\partial K(T_{n1l}^{j})} + \frac{\partial F}{\partial K(T_{n1l}^{j})} + \frac{\partial F}{\partial K(T_{nil}^{j})} + \frac{\partial F}{\partial K(T_{nil}^{j})} \right) + \\ &+ \sum_{n=1}^{N-1} \sum_{i=1}^{I-1} \left( \frac{\partial F}{\partial K(T_{ni0}^{j})} + \frac{\partial F}{\partial K(T_{ni1}^{j})} + \frac{\partial F}{\partial K(T_{ni1}^{j})} + \frac{\partial F}{\partial K(T_{nil}^{j})} + \frac{\partial F}{\partial K(T_{nil}^{j})} \right) \right], \quad (m = \overline{0, M}) \end{split}$$

$$X_{rqs}^g, X_{rqs}^{g+1/3}, X_{rqs}^{g+2/3}$$
 are calculated using the same formulas as in the first variational problem

$$\frac{\partial F}{\partial K(T_{0il}^{j})} = \frac{\partial F}{\partial K(T_{1il}^{j})} = \widetilde{A}_{il}^{j} \left( T_{1il}^{j} - T_{0il}^{j} \right) \qquad \qquad \frac{\partial F}{\partial K(T_{Nil}^{j})} = \frac{\partial F}{\partial K(T_{N-1,il}^{j})} = \widetilde{B}_{il}^{j} \left( T_{Nil}^{j} - T_{N-1,il}^{j} \right)$$

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## Necessary conditions for non-uniqueness of solution of the inverse problem

Let 
$$Y(x,t) \in C^{2,1}_{x,t}(G) \cap C^1(\overline{G})$$
  
be a solution of the direct problem (1)–(3)  
for two admissible thermal conductivities  
 $K_1(T) \in C^1([a,b])$  and  $K_2(T) \in C^1([a,b])$   $T \in [a,b]$   
Then the following assertions are true:

(a) There exists a function  $R(T) \in C([a,b])$  such that  $\Delta_x Y(x,t) = R(Y(x,t)) \cdot |\nabla_x Y(x,t)|^2$ 

(b) For such a function Y(x,t) the inverse problem has infinitely many solutions K(T)

The gradient of the cost functional is distributed over temperature strongly nonuniformly, which noticeably deteriorates the convergence of the iterative process.

This difficulty in solving the problem can be effectively overcome by applying an approach based on a sequential increase in the number M of partitions of the interval [a,b].

It is desirable to begin the process with M=1. After an optimal solution has been obtained, it is used as an initial approximation for the variant with M=2. The optimal solution found for M=2 is used as an initial approximation for M=4, etc.

## Analyze of the distribution of experimental data

It is concluded that the thermal conductivity is more effectively determined in the temperature range, which corresponds to a larger number of experimental data.

If it is important to determine the thermal conductivity in a particular temperature interval, then the experimental data in which the temperature belongs to the desired interval should be used.

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# Two criteria were used to evaluate the accuracy of the obtained numerical solutions of the inverse problem:

$$\varepsilon_{1} = \max_{0 \leq m \leq M} \frac{\left| K_{opt}(\widetilde{T}_{m}) - K(\widetilde{T}_{m}) \right|}{K^{*}} \qquad \qquad \varepsilon_{2} = \frac{1}{K^{*}} \sqrt{\sum_{m=0}^{M} \frac{\left( K_{opt}(\widetilde{T}_{m}) - K(\widetilde{T}_{m}) \right)^{2}}{M+1}}$$

 $K(\widetilde{T}_m)$  – the values of the analytical thermal conductivity coecient

 $K_{opt}(\widetilde{T}_m)$  – the obtained values of the optimal control

$$K^* = \frac{\sum_{m=0}^{M} K(\widetilde{T}_m)}{M+1} - \text{characteristic value}$$

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#### RESULTS OF NUMERICAL CALCULATIONS

The traces of the function  $\Lambda(x,y,z,t)$  were chosen as the initial function  $w_0(x,y,z)$  and as the boundary function  $w_\Gamma(x,y,z,t)$  on the parabolic boundary of the domain  $Q\times(0,\Theta)=(0,1)\times(0,1)\times(0,1)\times(0,1)$ . C(s)=1

#### **Experimental data:**

"Field" functional 
$$\beta(s(\Gamma)) = 0$$

The temperature field obtained as a result of solving a direct problem with a given thermal conductivity coefficient

"Flux" functional 
$$\mu(x, y, z, t) \equiv 0$$

The "experimental" heat flux on the surface of the parallelepiped was determined by the temperature field obtained as a result of solving a direct problem with a given thermal conductivity coefficient.

### The first series of computations

$$\Lambda(x, y, z, t) = x + y + z + 3t + 0.5 \tag{1}$$

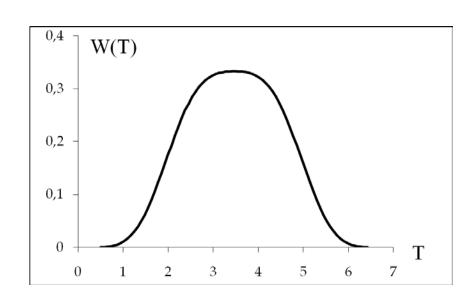
(1) is a solution of the direct problem for C(s) = 1, K(T) = T.

$$a = 0.5$$
  $b = 6.5$ 

Experimental data:  $Y_{nil}^{j} = \Lambda(x_n, y_i, z_{l,t}^{j}) = x_n + y_i + z_l + 3t^{j} + 0.5$ 

 $\Lambda(x,y,z,t)$  - a linear combination of spatial coordinates and time Therefore, the inverse problem may have a non-unique solution.

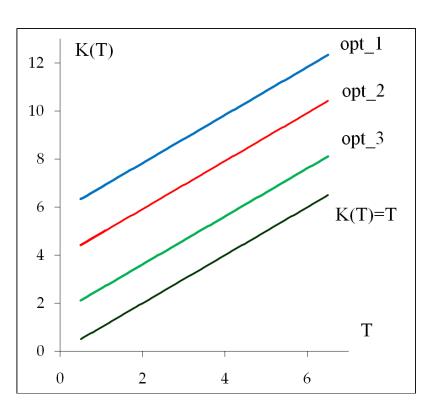
## Distribution of experimental data



$$K_{ini}(T) = 9.0 - opt \_1$$

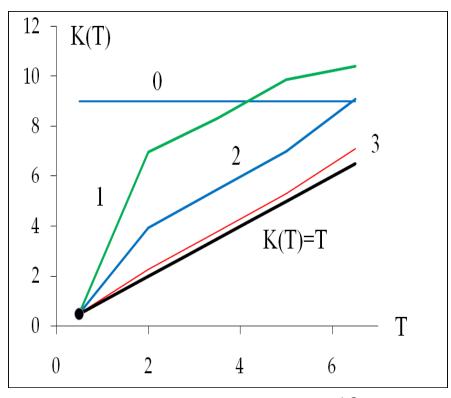
$$K_{ini}(T) = 7.0 - opt_2$$

$$K_{ini}(T) = 4.5 - opt_3$$



$$K_{opt}(T) = T + Const$$

In order to identify the only solution of the inverse problem, it is proposed to additionally set the point at which the desired thermal conductivity coefficient is known.



$$\varepsilon_1 = 5.1 \cdot 10^{-13}$$

# М

# The second series of computations

The traces of the function 
$$\Lambda(x, y, z, t) = \sqrt{\frac{x^2 + y^2 + z^2}{9 - 8t}}$$
 (2)

were chosen as the initial function  $w_0(x, y, z)$  and as the boundary function  $w_{\Gamma}(x, y, z, t)$  on the parabolic boundary of the domain  $Q \times (0, \Theta) = (0,1) \times (0,1) \times (0,1) \times (0,1)$ .

 $\Lambda(x, y, z, t)$  is a solution of the direct problem for C(s) = 1,  $K(T) = T^2$ 

$$a = 0.0$$
  $b = 1.732$ 

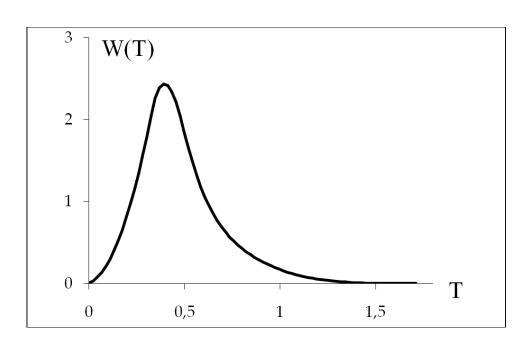
Experimental data:  $Y_{nil}^{j} = \Lambda(x_{n}, y_{i}, z_{l}, t^{j}) = \sqrt{\frac{x_{n}^{2} + y_{i}^{2} + z_{l}^{2}}{9 - 8t^{j}}}$ 

# м

#### Distribution of experimental data on [0.0, 1.732]

$$M = 64$$

$$N = I = L = 25$$



There is very little "experimental" data at the right end of the temperature interval at T>1.624.

The thermal conductivity coefficient is identified only on the temperature interval [0.0, 1.624].

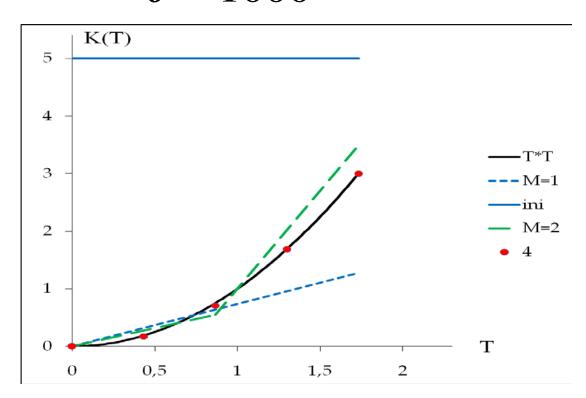
The trace of the selected initial approximation is saved on the segment [1.624, 1.732].

$$N = I = L = 25$$

$$J = 1000$$

$$(K_{ini}(T) \equiv 5.0)$$

$$M = 64$$



On the temperature interval [0.0, 1.624]

$$\varepsilon_1 = 1.6252 \cdot 10^{-3}$$
  $\varepsilon_2 = 8.4366 \cdot 10^{-4}$ 

# The third series of computations

The traces of the function

$$\Lambda(x, y, z, t) = \frac{3}{1.8 \cdot (5 - x - y - z - 1.8t)}$$
(3)

were chosen as the initial function  $w_0(x,y,z)$  and as the boundary function  $w_\Gamma(x,y,z,t)$  on the parabolic boundary of the domain

$$Q \times (0, \Theta) = (0,1) \times (0,1) \times (0,1) \times (0,1).$$

 $\Lambda(x, y, z, t)$  is a solution of the direct problem for C(s) = 1,  $K(T) = \frac{1}{T}$  a = 0.333 b = 8.333

Experimental data: 
$$Y_{nil}^{j} = T(x_n, y_i, z_{l,t}^{j}) = \frac{3}{1.8(5 - x_n - y_i - z_l - 1.8t^{j})}$$

 $\Lambda(x,y,z,t)$  - a linear combination of spatial coordinates and time

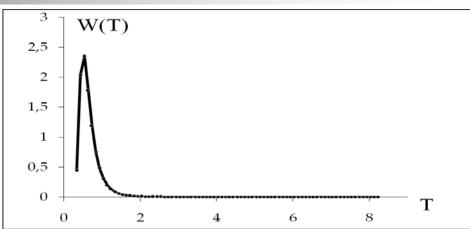
Therefore, the inverse problem may have a non-unique solution.

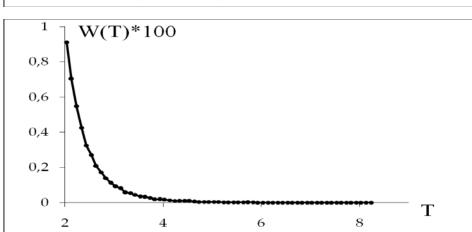


$$M = 80$$

# Distribution of experimental data on [0.333, 8.333]

# Distribution of experimental data on [2.0, 8.333]





There is very little "experimental" data at the right end of the temperature interval at T>6.

The thermal conductivity coefficient is identified only on the temperature interval [0.333, 6.0].

The trace of the selected initial approximation is saved on the segment [6.0, 8.333].

## The inverse problem has infinitely many solutions

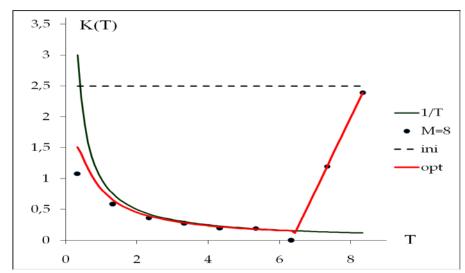
$$K_{opt}(T) = \frac{1}{T} + \frac{Const}{T^2}$$

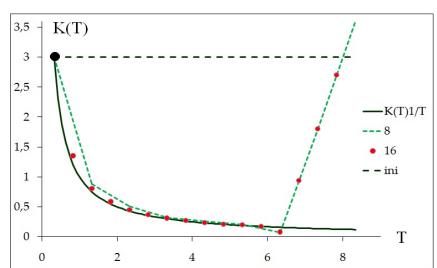
1. We don't keep the point

$$N = I = L = 25$$
$$J = 100$$

We set the point at which the thermal conductivity coefficient is known

$$M = 80$$



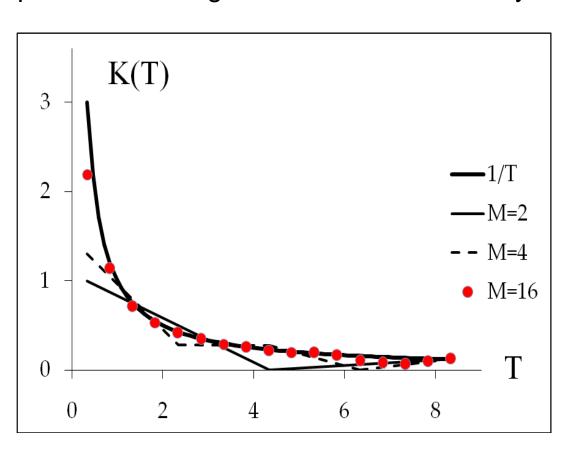




#### Flux functional

$$\mu(x, y, t) = 0, \quad \beta(s(\Gamma)) > 0$$

The "experimental" heat flux on the surface of the parallelepiped was determined by the temperature field obtained as a result of solving a direct problem with a given thermal conductivity coefficient.



The proposed algorithm leads to the same optimal solution regardless of which function is chosen as the initial approximation.

On the temperature interval [0.333, 6.0]

$$\varepsilon_1 = 3.5506 \cdot 10^{-4}$$

$$\varepsilon_2 = 1.5300 \cdot 10^{-4}$$

# М

## The fourth series of computations

The traces of the function

$$\Lambda(x, y, z, t) = \sqrt{\frac{9 \cdot (x+1)^2 + 20y^2 + 25z^2}{9 - 8t}}$$
(4)

were chosen as the initial function  $w_0(x, y, z)$  and as the boundary function  $w_{\Gamma}(x, y, z, t)$  on the parabolic boundary of the domain

$$Q \times (0, \Theta) = (0,1) \times (0,1) \times (0,1) \times (0,1)$$
.

As the experimental field Y(x; y; z; t) was chosen the temperature field, which was obtained as a result of solving the direct problem at C(s) = 1 and with the thermal conductivity coecient K(T) = k(T), where the function k(T) is determined by the equality:

the equality: 
$$k(T) = \begin{cases} 0.1 \cdot (T-3) \cdot (T-6) \cdot (T-7) + 3.4, & T \ge 3, \\ 1.2 \cdot (T-3) + 3.4, & T < 3. \end{cases}$$
  $a = 1.0$   $b = 9.0$ 

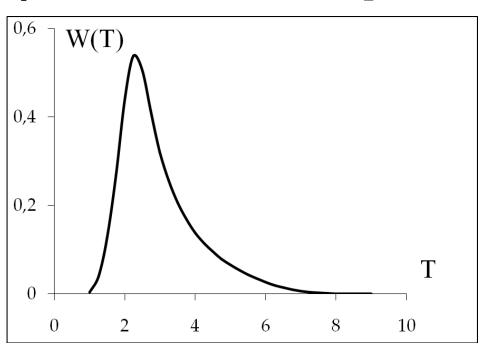
# М

#### Distribution of experimental data on [1.0, 9.0]

$$M = 64$$

$$N = I = L = 25$$

$$J = 25$$



There is very little "experimental" data at the right end of the temperature interval at T>8.0.

The trace of the selected initial approximation is saved on the segment [8.0, 9.0].



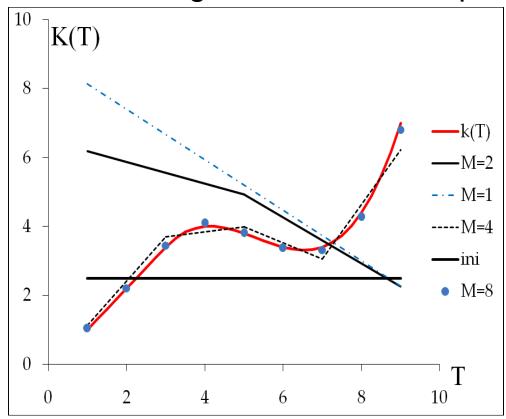
#### **Field functional**

$$\beta(s(\Gamma)) = 0$$

1. 
$$\mu(x, y, z, t) \equiv 1$$

The control functions at dierent stages of the iterative process

$$K_{ini}(T) = 2.5$$

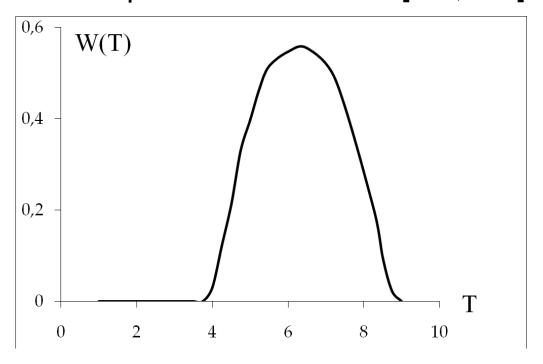


On the temperature interval [1.0, 8.0]

$$\varepsilon_1 = 7.2876 \cdot 10^{-6}$$
  $\varepsilon_2 = 1.5006 \cdot 10^{-6}$ 

2. 
$$\mu_{nil}^{j} = \begin{cases} 1, & x[n] + y[i] + z[l] + t[j] \ge 3.5 \\ 0, & \textit{в остальных точках.} \end{cases}$$

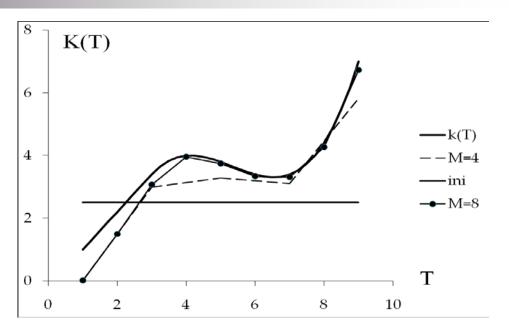
#### Distribution of experimental data on [1.0, 9.0]



Here most of the "experimental" data is concentrated on the interval [4.0, 9.0]. However, there are practically no "experimental" data at T < 4.0.



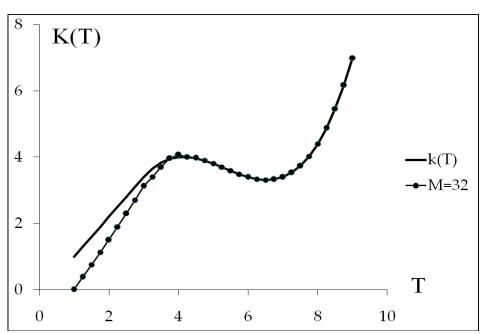
# The control functions at different stages of the iterative process



On the temperature interval [4.0, 9.0]

$$\varepsilon_1 = 3.6520 \cdot 10^{-3}$$

$$\varepsilon_2 = 1.1316 \cdot 10^{-3}$$



3. 
$$\mu_{nil}^{j} = \begin{cases} 1, & n, i, l = 3, 7, 11, 15, 19, 23, \\ 0, & in other cases. \end{cases}$$

(216 "control" points in the functional)

Distribution of experimental data on [1.0, 9.0] and the convergence process are the same as in the first case

$$\varepsilon_1 = 8.8594 \cdot 10^{-6}$$

$$\varepsilon_2 = 1.6499 \cdot 10^{-6}$$

$$\mu_{nil}^{j} = \begin{cases} 1, & i \leq 3, \\ 0, & in other cases. \end{cases}$$

Distribution of experimental data on [1.0, 9.0] and the convergence process are the same as in the first case

$$\varepsilon_1 = 3.6477 \cdot 10^{-2}$$

$$\varepsilon_2 = 6.7738 \cdot 10^{-3}$$



A task of special interest is to compare the thermal conductivity coefficients obtained in two different formulations of the identification problem, namely, "field" functional and "flux" functional.

The solution of the problem may be nonunique in the former case, whereas an analysis of numerous problems in the latter case has never revealed the nonuniqueness of the solution.

An additional argument for using the flux functional in determining the thermal conductivity is that the heat flux on the boundary of the object is easier to measure than the temperature in the object.

#### Stability of the solutions

- 1) The proposed algorithm has demonstrated its stability: Small deviations in the experimental data (~10%) lead to errors in the solution of the same order (~2-5%) (  $\epsilon = 0$  ).
- 2) To reduce oscillations in the solution of the inverse problem in the case when the perturbations in the input data are not small (20 30%), it is advisable to use smoothing term in the cost functional  $\varepsilon > 0$ .
- 3) If the perturbations in the input data are not small, then you can achieve the smoothing solution by choosing a small number M of partitions of the interval [a, b].
- 4) For the efficient work of the proposed algorithm it is advisable to solve the inverse problem beginning from small values of M. The obtained solution is used as the initial approximation for larger values of M.

# Thank you for your attention!