The FAD-methodology and Recovery the Thermal Conductivity Coefficient in Two Dimension Case

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Abstract

The problem of determining the thermal conductivity coefficient that depends on temperature is studied. The consideration is based on the Dirichlet boundary value problem for the two-dimensional unsteady-state heat equation. The inverse coefficient problem is reduced to a variation problem. The mean-root-square deviations of the temperature field from the experimental data is used as the objective functional. An algorithm for the numerical solution of the inverse coefficient problem is proposed. It is based on the modern approach of Fast Automatic Differentiation technique, which made it possible to solve a number of difficult optimal control problems for dynamic systems. An expression for the gradient of the objective functional is obtained for the discrete optimal control problem. The examples of solving the inverse coefficient problem confirm the efficiency of the proposed algorithm.

Introduction

In the description and mathematical modeling of many thermal processes, the classical heat equation is often used. The density of the substance, its specific thermal capacity, and the thermal conductivity coefficient appearing in this equation are assumed to be known functions of the coordinates and temperature. Additional boundary conditions make it possible to determine the dynamics of the temperature field in the substance under examination.

However, the substance properties are not always known. It often happens that the thermal conductivity coefficient depends only on the temperature, and this dependence is not known. In this case, the problem of determining the dependence of the thermal conductivity coefficient on the temperature based on experimental measurements of the temperature field arises. This problem also arises when a complex thermal process should be described by a simplified mathematical model. For example, in studying and modeling heat propagation in complex porous composite materials, where the radiation heat transfer plays a considerable role, both the

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convective and radiative heat transfer must be taken into account. The thermal conductivity coefficients in this case typically depend on the temperature. To estimate these coefficients, various models of the medium are used. As a result, one has to deal with a complex nonlinear model that describes the heat propagation in the composite material (see [Alifanov & Cherepanov, 2009]). However, another approach is possible: a simplified model is constructed in which the radiative heat transfer is not taken into account, but its effect is modeled by an effective thermal conductivity coefficient that is determined based on experimental data.

In [Zubov, 2016] the inverse coefficient problems are studied for the one-dimensional unsteady-state heat equation. There was considered the case of continuous thermal conductivity coefficient. In [Albu et al., 2017] the case of a discontinuous thermal conductivity coefficient is investigated.

In this paper we consider the problem studied in [Zubov, 2016] for the two-dimensional unsteady-state heat equation. The inverse coefficient problem is reduced to a variation problem. The mean-root-square deviation of the temperature field is used as the objective functional. An algorithm for the numerical solution of the inverse coefficient problem is proposed. It is based on the using of Fast Automatic Differentiation technique.

1 Formulation of the Problem

A layer of material of length L and width R is considered. The temperature of this layer at the initial time is given. It is also known how the temperature on the boundary of this layer changes in time. The distribution of the temperature field at each instant of time is described by the following initial boundary value (mixed) problem:

$$\rho C \frac{\partial T(x,y,t)}{\partial t} = \frac{\partial}{\partial x}\left(K(T)\frac{\partial T(x,y,t)}{\partial x}\right) + \frac{\partial}{\partial y}\left(K(T)\frac{\partial T(x,y,t)}{\partial y}\right), \qquad (1)$$
$$(x,y) \in Q = [0,L] \times [0,R], \qquad t \in [0,\Theta],$$

$$\begin{aligned}
T(x,y,0) &= w_0(x,y), && (x,y) \in Q, && (2)\\
T(0,y,t) &= w_1(y,t), && 0 \le y \le R, \quad 0 \le t \le \Theta, && (3)\\
T(L,y,t) &= w_2(y,t), && 0 \le y \le R, \quad 0 \le t \le \Theta, && (4)\\
T(x,0,t) &= w_3(x,t), && 0 \le x \le L, \quad 0 \le t \le \Theta, && (5)\\
T(x,R,t) &= w_4(x,t), && 0 \le x \le L, \quad 0 \le t \le \Theta. && (6)
\end{aligned}$$

Here (x,y) are the Cartesian coordinates of the point in the layer; t is the time; $T(x,y,t)$ is the temperature of the material at the point with the coordinates (x,y) at the time t; ρ and C are the density and the heat capacity of the material, respectively; $K(T)$ is the thermal conductivity coefficient; $w_0(x,y)$ is the given temperature of the layer at the initial time; $w_1(y,t)$ and $w_2(y,t)$ are the given temperatures for $x=0$ and for $x=L$ respectively; $w_3(x,t)$ and $w_4(x,t)$ are the given temperatures for $y=0$ and for $y=R$ respectively.

If the dependence of the thermal conductivity coefficient $K(T)$ on the temperature T is known, then we can solve the mixed problem (1)–(6) to find the temperature distribution $T(x,y,t)$ in $Q \times [0,\Theta]$. Below, problem (1)–(6) will be called the direct problem.

If the dependence of the thermal conductivity coefficient on the temperature is not known, it is of interest to determine this dependence. A possible statement of this problem (it is classified as a model's parameters identification problem) is as follows: find the dependence $K(T)$ on T under which the temperature field $T(x,y,t)$ obtained by solving problem (1)–(6) is close to the field $Y(x,y,t)$ obtained experimentally. The quantity

$$\Phi(K(T)) = \int_0^\Theta \int_0^L \int_0^R \left[T(x,y,t) - Y(x,y,t)\right]^2 \cdot \mu(x,y,t)\,dx\,dy\,dt \qquad (7)$$

may be used as the measure of difference between these functions. Here $\mu(x,y,t) \ge 0$ is a given weighting function.

Thus, the optimal control problem is to find the optimal control $K(T)$ and the corresponding optimal solution $T(x,y,t)$ of problem (1)–(6) that minimizes functional (7).

2 Finding the Gradient of Functional

The optimal control problem formulated above was solved numerically. The objective functional was minimized using the gradient method. It is well known that it is very important for the gradient methods to determine accurate values of the gradients. For this reason, in this paper we used the efficient Fast Automatic Differentiation technique ([Evtushenko, 1998]) to calculate the components of the functional gradient. The unknown function $K(T)$ was approximated by a continuous piecewise linear function.

One of the main elements of the proposed numerical method is the solution of the mixed problem (1)–(6). To this end, the domain $[0,L]\times[0,R]\times[0,\Theta]$ is decomposed by the grid lines $\{x_n\}_{n=0}^{N}$, $\{y_i\}_{i=0}^{I}$, and $\{t^j\}_{j=0}^{J}$ into parallelepipeds. At each node (x_n, y_i, t^j) characterized by the indices (n,i,j), all the functions are determined by their values at the point (x_n, y_i, t^j) (e.g., $T(x_n, y_i, t^j) = T_{ni}^j$). In each parallelepiped, the thermal balance must be preserved. As a result, using two-layer implicit scheme with weights we obtain the following finite difference scheme that approximates the mixed problem (1)–(6):

$$\begin{aligned}
S_{ni}\cdot\rho C(T_{ni}^{j+1}-T_{ni}^{j}) &= \sigma\tau^j A(T^{j+1}) + (1-\sigma)\tau^j A(T^j), \qquad (n=\overline{1,N-1},\ i=\overline{0,I-1},\ j=\overline{1,J}), && (8)\\
T_{ni}^0 &= (w_0)_{ni}, \qquad (n=\overline{0,N},\ i=\overline{0,I}), && (9)\\
T_{0i}^j &= (w_1)_i^j, \qquad (i=\overline{0,I},\ j=\overline{1,J}), && (10)\\
T_{Ni}^j &= (w_2)_i^j, \qquad (i=\overline{0,I},\ j=\overline{1,J}), && (11)\\
T_{n0}^j &= (w_3)_n^j, \qquad (n=\overline{0,N},\ j=\overline{1,J}), && (12)\\
T_{nI}^j &= (w_4)_n^j, \qquad (n=\overline{0,N},\ j=\overline{1,J}). && (13)
\end{aligned}$$

Here σ is the weight parameter,

$$\begin{aligned}
A(T^j) &= \frac{K(T_{n+1,i}^j)+K(T_{ni}^j)}{2}\cdot\frac{T_{n+1,i}^j-T_{ni}^j}{h_n^x}\cdot(\tilde y_{i+1}-\tilde y_i) - \frac{K(T_{ni}^j)+K(T_{n-1,i}^j)}{2}\cdot\frac{T_{ni}^j-T_{n-1,i}^j}{h_{n-1}^x}\cdot(\tilde y_{i+1}-\tilde y_i) +\\
&+ \frac{K(T_{n,i+1}^j)+K(T_{ni}^j)}{2}\cdot\frac{T_{n,i+1}^j-T_{ni}^j}{h_i^y}\cdot(\tilde x_{n+1}-\tilde x_n) - \frac{K(T_{ni}^j)+K(T_{n,i-1}^j)}{2}\cdot\frac{T_{ni}^j-T_{n,i-1}^j}{h_{i-1}^y}\cdot(\tilde x_{n+1}-\tilde x_n),\\
h_n^x &= x_{n+1}-x_n, \quad (n=\overline{0,N-1}), \qquad h_i^y = y_{i+1}-y_i, \quad (i=\overline{0,I-1}),\\
\tau^j &= t^j - t^{j-1}, \quad (j=\overline{1,J}),\\
\tilde x_0 &= x_0; \quad \tilde x_n = x_{n-1}+h_{n-1}^x/2; \quad n=\overline{1,N}; \quad \tilde x_{N+1} = x_N;\\
\tilde y_0 &= y_0; \quad \tilde y_i = y_{i-1}+h_{i-1}^y/2; \quad i=\overline{1,I}; \quad \tilde y_{I+1} = y_I;\\
S_{ni} &= (\tilde x_{n+1}-\tilde x_n)(\tilde y_{i+1}-\tilde y_i).
\end{aligned}$$

The system of nonlinear algebraic equations (8)–(13) was solved iteratively using the method:

$$\overset{s}{T}{}_{ni}^{j+1} = \frac{\sigma\tau^j}{S_{ni}\cdot\rho C}\,A\left(\overset{s-1}{T}{}^{j+1}\right) + \frac{(1-\sigma)\tau^j}{S_{ni}\cdot\rho C}\,A\left(T^j\right) + T_{ni}^j, \qquad \text{where } \overset{0}{T}{}_{ni}^{j+1} = T_{ni}^j.$$

This approach was used in the work to solve the mixed problem (1)–(6), and the function $T(x,y,t)$ (more precisely, its approximation T_{ni}^j) was found.

The temperature interval $[a,b]$ (the interval of interest) is partitioned by the points $\widetilde T_0 = a, \widetilde T_1, \widetilde T_2, \ldots, \widetilde T_M = b$ into M parts (they can be equal or of different lengths). Each point $\widetilde T_m$ $(m=0,\ldots,M)$ is assigned a number $k_m = K(\widetilde T_m)$. The function $K(T)$ to be found is approximated by a continuous piecewise linear function with the nodes at the points $\left\{(\widetilde T_m, k_m)\right\}_{m=0}^{M}$ so that

$$K(T) = k_{m-1} + \frac{k_m - k_{m-1}}{\widetilde T_m - \widetilde T_{m-1}}(T - \widetilde T_{m-1}) \qquad \text{for } \widetilde T_{m-1} \le T \le \widetilde T_m, \qquad (m=1,\ldots,M).$$

The objective functional (7) was approximated by a function $F(k_0, k_1, \ldots, k_M)$ of the finite number of variables as

$$\Phi(K(T)) \approx F = \sum_{j=1}^{J}\sum_{i=1}^{I-1}\sum_{n=1}^{N-1}\left((T_{ni}^j - Y_{ni}^j)^2\cdot\mu_{ni}^j h_n^x h_i^y \tau^j\right).$$

According to [Evtushenko, 1998], approximation (8)-(13) of the mixed problem (1)-(6) is reduced to the canonical form

$$\begin{aligned}
T_{ni}^{j+1} &= T_{ni}^j + a_{ni}^j \left(K(T_{n+1,i}^j) + K(T_{ni}^j)\right) \cdot \left(T_{n+1,i}^j - T_{ni}^j\right) - \tilde{a}_{ni}^j \left(K(T_{ni}^j) + K(T_{n-1,i}^j)\right) \cdot \left(T_{ni}^j - T_{n-1,i}^j\right) + \\
&+ b_{ni}^j \left(K(T_{ni}^j) + K(T_{n,i+1}^j)\right) \cdot \left(T_{n,i+1}^j - T_{ni}^j\right) - \tilde{b}_{ni}^j \left(K(T_{ni}^j) + K(T_{n,i-1}^j)\right) \cdot \left(T_{ni}^j - T_{n,i-1}^j\right) + \\
&+ c_{ni}^j \left(K(T_{n+1,i}^{j+1}) + K(T_{ni}^{j+1})\right) \cdot \left(T_{n+1,i}^{j+1} - T_{ni}^{j+1}\right) - \tilde{c}_{ni}^j \left(K(T_{ni}^{j+1}) + K(T_{n-1,i}^{j+1})\right) \cdot \left(T_{ni}^{j+1} - T_{n-1,i}^{j+1}\right) + \\
&+ d_{ni}^j \left(K(T_{ni}^{j+1}) + K(T_{n,i+1}^{j+1})\right) \cdot \left(T_{n,i+1}^{j+1} - T_{ni}^{j+1}\right) - \tilde{d}_{ni}^j \left(K(T_{ni}^{j+1}) + K(T_{n,i-1}^{j+1})\right) \cdot \left(T_{ni}^{j+1} - T_{n,i-1}^{j+1}\right) \equiv \psi_{ni}^j, \\
&(n = \overline{1, N-1}, \qquad i = \overline{0, I-1}, \qquad j = \overline{1, J}),
\end{aligned}$$

where the notations

$$\begin{aligned}
a_{ni}^j &= \frac{(1-\sigma)\tau^j(\tilde{y}_{i+1} - \tilde{y}_i)}{2S_{ni} \cdot \rho C h_n^x}, \qquad \tilde{a}_{ni}^j = \frac{(1-\sigma)\tau^j(\tilde{y}_{i+1} - \tilde{y}_i)}{2S_{ni} \cdot \rho C h_{n-1}^x}, \qquad b_{ni}^j = \frac{(1-\sigma)\tau^j(\tilde{x}_{n+1} - \tilde{x}_n)}{2S_{ni} \cdot \rho C h_i^y}, \\
\tilde{b}_{ni}^j &= \frac{(1-\sigma)\tau^j(\tilde{x}_{n+1} - \tilde{x}_n)}{2S_{ni} \cdot \rho C h_{i-1}^y}, \qquad c_{ni}^j = \frac{\sigma\tau^j(\tilde{y}_{i+1} - \tilde{y}_i)}{2S_{ni} \cdot \rho C h_n^x}, \qquad \tilde{c}_{ni}^j = \frac{\sigma\tau^j(\tilde{y}_{i+1} - \tilde{y}_i)}{2S_{ni} \cdot \rho C h_{n-1}^x}, \\
d_{ni}^j &= \frac{\sigma\tau^j(\tilde{x}_{n+1} - \tilde{x}_n)}{2S_{ni} \cdot \rho C h_i^y}, \qquad \tilde{d}_{ni}^j = \frac{\sigma\tau^j(\tilde{x}_{n+1} - \tilde{x}_n)}{2S_{ni} \cdot \rho C h_{i-1}^y} \qquad \text{are used.}
\end{aligned}$$

The Fast Automatic Differentiation technique makes it possible to formally write relations determining the adjoint problem of (8)-(13) for the conjugate variables p_i^j, $(n = \overline{1, N-1},\ i = \overline{0, I-1},\ j = \overline{1, J})$:

$$\begin{aligned}
p_{ni}^j &= p_{ni}^{j+1} + \{a_{ni}^j \cdot X_{ni}^j - \tilde{a}_{ni}^j \cdot Y_{ni}^j + b_{ni}^j \cdot U_{ni}^j - \tilde{b}_{ni}^j \cdot V_{ni}^j\} \cdot p_{ni}^{j+1} + a_{n-1,i}^j \cdot Y_{ni}^j \cdot p_{n-1,i}^{j+1} - \\
&- \tilde{a}_{n+1,i}^j \cdot X_{ni}^j \cdot p_{n+1,i}^{j+1} + b_{n,i-1}^j \cdot V_{ni}^j \cdot p_{n,i-1}^{j+1} - \tilde{b}_{n,i+1}^j \cdot U_{ni}^j \cdot p_{n,i+1}^{j+1} + \\
&+ \{c_{ni}^{j-1} \cdot X_{ni}^j - \tilde{c}_{ni}^{j-1} \cdot Y_{ni}^j + d_{ni}^{j-1} \cdot U_{ni}^j - \tilde{d}_{ni}^{j-1} \cdot V_{ni}^j\} \cdot p_{ni}^j + c_{n-1,i}^{j-1} \cdot Y_{ni}^j \cdot p_{n-1,i}^j - \\
&- \tilde{c}_{n+1,i}^{j-1} \cdot X_{ni}^j \cdot p_{n+1,i}^j + d_{n,i-1}^j \cdot V_{ni}^j \cdot p_{n,i-1}^j - \tilde{d}_{n,i+1}^{j-1} \cdot U_{ni}^j \cdot p_{n,i+1}^j + \frac{\partial F}{\partial T_{ni}^j},
\end{aligned}$$

where

$$\begin{aligned}
X_{ni}^j &= K'(T_{ni}^j) \cdot (T_{n+1,i}^j - T_{ni}^j) - K(T_{ni}^j) - K(T_{n+1,i}^j), \\
Y_{ni}^j &= K'(T_{ni}^j) \cdot (T_{ni}^j - T_{n-1,i}^j) + K(T_{ni}^j) + K(T_{n-1,i}^j), \\
U_{ni}^j &= K'(T_{ni}^j) \cdot (T_{n,i+1}^j - T_{ni}^j) - K(T_{ni}^j) - K(T_{n,i+1}^j), \\
V_{ni}^j &= K'(T_{ni}^j) \cdot (T_{ni}^j - T_{n,i-1}^j) + K(T_{ni}^j) + K(T_{n,i-1}^j), \\
K'(T_{ni}^j) &= \frac{\partial K(T)}{\partial T}(T_{ni}^j) = \begin{cases} \dfrac{k_{m+1} - k_m}{\widetilde{T}_{m+1} - \widetilde{T}_m}, & \text{if } \widetilde{T}_m \le T_{ni}^j \le \widetilde{T}_{m+1}, \\ 0, & \text{otherwise.} \end{cases}
\end{aligned}$$

We assume that $p_{ni}^{J+1} = 0$, $p_{0i}^j = p_{Ni}^j = p_{n0}^j = p_{nI}^j = 0$; $n = \overline{1, N}$, $i = \overline{1, I}$, $j = \overline{1, J}$.

According to the Fast Automatic Differentiation technique, the components of the gradient of the objective function are calculated by the formula:

$$\frac{\partial F}{\partial k_m} = \sum_{g=0}^{J} \sum_{r=0}^{I} \sum_{l=0}^{N} \left(\sum_{j=1}^{J} \sum_{i=1}^{I-1} \sum_{n=1}^{N-1} \frac{\partial \psi_{ni}^j}{\partial K(T_{lr}^g)} \cdot p_{ni}^j \right) \cdot \frac{\partial K(T_{lr}^g)}{\partial k_m}, \qquad m = \overline{0, M}. \tag{14}$$

The factors $\dfrac{\partial K(T_{lr}^g)}{\partial k_m}$ that appear in (14) are calculated by the formulas

$$\frac{\partial K(T_{ni}^j)}{\partial k_m} = \begin{cases} 1 - \dfrac{T_{ni}^j - \widetilde{T}_m}{\widetilde{T}_{m+1} - \widetilde{T}_m}, & \text{if } \widetilde{T}_m \le T_{ni}^j \le \widetilde{T}_{m+1}, \\ 0, & \text{otherwise.} \end{cases} \qquad \frac{\partial K(T_{ni}^j)}{\partial k_{m+1}} = \begin{cases} \dfrac{T_{ni}^j - \widetilde{T}_m}{\widetilde{T}_{m+1} - \widetilde{m}_n}, & \text{if } \widetilde{T}_m \le T_{ni}^j \le \widetilde{T}_{m+1}, \\ 0, & \text{otherwise.} \end{cases}$$

The value of the gradient of the objective function $F(k_0, k_1, \ldots, k_M)$ calculated by formula (14) is exact for the chosen approximation of the optimal control problem.

The function $F(k_0, k_1, \ldots, k_M)$ was minimized numerically using the gradient method.

3 Numerical Results

To illustrate the efficiency of the proposed algorithm the following variation problem was considered:

$$\begin{aligned}
\frac{\partial T(x,y,t)}{\partial t} &= \frac{\partial}{\partial x}\left(K(T)\frac{\partial T(x,y,t)}{\partial x}\right) + \frac{\partial}{\partial y}\left(K(T)\frac{\partial T(x,y,t)}{\partial y}\right), \qquad (x,y) \in Q, \qquad t > 0,\\
T(x,y,0) &= x^2 + 7xy - y^2 + \sin\left(\frac{\pi}{2}x\right) \cdot \sin(2\pi y), \qquad (0 \le x \le 2, \quad 0 \le y \le 1),\\
T(0,y,t) &= -y^2, \qquad T(2,y,t) = 14y - y^2 + 4, \qquad (t \ge 0, \quad 0 \le y \le 1),\\
T(x,0,t) &= x^2, \qquad T(x,1,t) = x^2 + 7x - 1, \qquad (t \ge 0, \quad 0 \le x \le 2).
\end{aligned}$$

Here $Q = \{(0 \le x \le 2) \times (0 \le y \le 1)\}$.

Note that the inverse problem with above-indicated data has an analytical solution; indeed, the function $Y(x,y,t) = x^2 + 7xy - y^2 + \exp(-t)\sin\left(\frac{\pi}{2}x\right) \cdot \sin(2\pi y)$ is the solution of the mixed problem (1)-(6) with the input data indicated above for $K(T) = \frac{4}{17\pi^2}$. In this case $a = -1$, $b = 17$.

To solve the direct and inverse problems, we used the uniform grid with the parameters $N = I = 150$ (the number of intervals along the axis x and y) and $J = 3400$ (the number of intervals along the axis t), which ensures the sufficient accuracy of computation of the temperature field. The interval $[a, b]$ was portioned into nine intervals ($M = 9$). The parameter σ was equal to 0.6 and $\mu(x,y,t) \equiv 1$.

The solution of the identification problem in this case is illustrated in Fig. 1. This figure shows the functions $K(T)$ at different steps of the iterative process. The line marked by the number 0 corresponds to the initial approximation to solution $K(T) \equiv 0.01$. The further approximations to the solution of the identification problem (finding function $K(T)$) are shown in several iterative steps and are marked by increasing numbers. Finally, the line marked by **opt** is a limiting one obtained after the completion of the iterative process. The results illustrated in Fig. 1 demonstrate the convergence of the approximate values of $K(T)$ to the limiting function $K(T) = \frac{4}{17\pi^2}$.

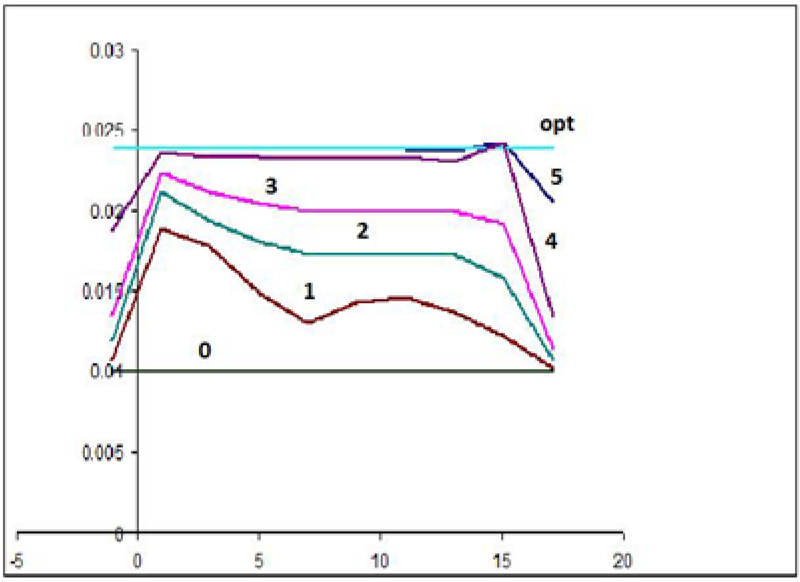

Figure 1: Different steps of the iterative process

In more details, the process of finding the thermal conductivity coefficient is as follows. If the experimental temperature field is determined by the solution of the direct problem with the given $K(T) = \frac{4}{17\pi^2}$, i.e., $Y^j_{ni} = T^j_{ni}$, then the objective functional changes from 1.53445×10^{-2} to 3.47387×10^{-30}, and the maximum of the gradient's absolute value decreases from 9.40155×10^{-1} to 1.71804×10^{-15}, while the coefficient of thermal conductivity coincides with $K(T) = \dfrac{4}{17\pi^2}$ accurate to the machine precision.

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