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On a posteriori pointwise error estimation using adjoint temperature and Lagrange remainder

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Abstract

The pointwise estimation of heat conduction solution as a function of truncation error of a finite difference scheme is addressed. The truncation error is estimated using a Taylor series with the remainder in the Lagrange form. The contribution of the local error to the total pointwise error is estimated via an adjoint temperature. It is demonstrated that the results of numerical calculation of the temperature at an observation point may thus be refined via adjoint error correction and that an asymptotic error bound may be found.

Keywords: Adjoint equation; Finite differences; Truncation error estimation

1. Introduction

At present, there are many numerical methods enabling a very accurate solution of the heat conduction equation. Nevertheless, an estimate of the error of a concrete calculation is performed relatively rarely. From an historical perspective this is due to the huge computational burden of numerical error calculation. The availability of ever increasing performance of computers has led to a significant raise in number of publications on this subject.

The Richardson extrapolation [24,32–34] is the most popular method for numerical error estimation and correction at present as far as finite-difference methods are concerned. Unfortunately, it becomes complicated for schemes containing differences with a mixed order of accuracy. Many other effects may change the

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nominal order of the grid convergence, for instance the presence of discontinuities [6–8,43]. Spatial nonuniformity of the grid may also reduce the convergence rate [43]. Thus, a correct use of Richardson extrapolation requires a set of grids to prove monotonous convergence and to determine real order of convergence for a given solution. This may turn to be very expensive from a computer resources viewpoint.

There exists an alternative approach for a posteriori error estimation based on the adjoint equations and residual estimation and aimed at estimating certain quantities of interest (goal-oriented methods) [1,10,9,8,20,26–31,39,40].

This approach was used in [10–18,39,40] for the refinement of practically useful functionals both by finite-element and finite-difference methods. The local truncation error (residual) was estimated through the action of a differential operator on the interpolated solution, while its contribution to the functional was calculated using an adjoint problem. The error is shown to be composed of two components, the first being computable using adjoint parameters and residual while the second is incomputable (depending on errors of solution of both primal and adjoint problems). In [39,40] information on spatial distribution of the residuals was used for mesh refining (for diminishing the incomputable error) above the estimation of the computable error.

In the present work we consider another approach for the estimation of computable error in finite differences if compared with [10]. It is based on a differential approximation (DA) [36] instead of being based on direct estimation of the residual. This provides for certain differences both in applicability domain and features of the methods. We use a local truncation error estimated from a Taylor series with the remainder in Lagrange form and adjoint equations in a continuous form. This enables us both to correct the error and to obtain an error bound for the refined solution. The refinement and the error bound are obtained on the same grid as that employed for the primal problem solution and require identical computer time.

2. Numerical error estimation using the adjoint temperature

Let us consider the estimation of the temperature error at a checkpoint for the finite-difference solving of the unsteady one dimensional heat conduction equation.

$$C\rho\frac{\partial \widetilde{T}}{\partial t} - \frac{\partial}{\partial x}\left(\lambda\frac{\partial \widetilde{T}}{\partial x}\right) = 0 \quad \text{in } Q = \Omega\times(0,t_f),\ \ \Omega \in R^1, \tag{1}$$

$$\text{Initial conditions:}\quad \widetilde{T}(0,x) = T_0(x);\quad T_0(x)\in L_2(\Gamma_i), \tag{2}$$

$$\text{Boundary conditions:}\quad \left.\frac{\partial \widetilde{T}}{\partial x}\right|_{x=0} = 0;\quad \left.\frac{\partial \widetilde{T}}{\partial x}\right|_{x=X} = 0. \tag{3}$$

Here C is the thermal capacity, λ is the thermal conductivity, ρ is the density, $\widetilde{T}$ is the temperature (considered here as exact, nonperturbed), x is the coordinate, X is the thickness, t is the time, t_f is the duration of process, Ω is the domain of calculation, ρ = Const, C = Const.

In this paper we shall consider two cases: λ = Const, $\widetilde{T}(t,x)\in C^\infty(Q)$ and $\lambda\in L_2(\Omega)$, $\widetilde{T}(t,x)\in H^1(Q)$. In these spaces the problem is well-posed [22].

Consider a finite-difference approximation of the first order in time and second order in space (for the constant λ), of Eq. (1) namely:

$$C\rho\frac{T_k^n - T_k^{n-1}}{\tau} - \lambda\frac{T_{k+1}^n - 2T_k^n + T_{k-1}^n}{h_k^2} = 0. \tag{4}$$

Here T is the approximate solution of finite difference equation, τ is the temporal step and h_k is the spatial stepsize.

The simplicity of the scheme and the low order of approximation are deliberately chosen to illustrate the features of this approach with the simplest mathematical treatment.

Let us expand the mesh function T_k^n in a Taylor series and substitute to (4). Herein we imply that there exists the smooth enough function $T(t,x)$ that coincides with T_k^n at all grid points. Then Eq. (4) transforms to Eq. (5) denoted as the differential approximation [24,36].

$$C\rho\frac{\partial T}{\partial t} - \lambda\frac{\partial^2 T}{\partial x^2} + \delta T = 0. \tag{5}$$

Here $\delta T = \delta T_t + \delta T_x$ is a local truncation error engendered by Taylor series remainders and again T is the approximate solution of finite difference equation (4) and

$$\delta T_t = -\frac{C\rho}{2}\tau\frac{\partial^2 T(t_n - \alpha_k^n\tau, x_k)}{\partial t^2}, \quad \delta T_x = -\frac{\lambda}{24}h_k^2\left(\frac{\partial^4 T(t_n, x_k + \beta_k^n h)}{\partial x^4} + \frac{\partial^4 T(t_n, x_k - \gamma_k^n h)}{\partial x^4}\right).$$

We use here the Lagrange form of remainder, which contains unknown parameters $\alpha_k^n, \beta_k^n, \gamma_k^n \in (0,1)$. The mathematical properties of differential approximations are discussed in [24,36]. According to [36] $T(t,x) \in C^\infty(Q)$.

Thus, when solving the finite difference equation (4) we deal with the differential approximation (5) instead of exact equation (1). The deviation of Eq. (5) from (1) is caused by the source term δT. By introducing an solution error ΔT ($T = \widetilde{T} + \Delta T$) we can reformulate (5) as

$$C\rho\frac{\partial(\widetilde{T} + \Delta T)}{\partial t} - \lambda\frac{\partial^2(\widetilde{T} + \Delta T)}{\partial x^2} + \delta T = 0. \tag{5a}$$

Herein, we address the impact of this disturbing source term on some quantities of interest for an example of temperature at certain checkpoint. The error of the temperature calculation at the checkpoint $T_{\text{est}} = T(t_{\text{est}}, x_{\text{est}})$ is determined by the sum of contributions of local truncation error with weights depending on the transfer of disturbances. For their determination let us denote the estimated temperature T_{est} by ε and express it as the functional

$$T_{\text{est}} = \varepsilon = \int\int_\Omega T(t,x)\delta(t - t_{\text{est}})\delta(x - x_{\text{est}})\,\mathrm{d}t\,\mathrm{d}x. \tag{6}$$

Here δ is Dirac's delta function.

The most efficient method for calculation of the functional variation is known to be based on adjoint equations. Let us use this approach here. For this purpose let us introduce a Lagrangian comprised of the estimated value and a weak statement of (5).

$$\begin{aligned} L = &\int\int_\Omega T(t,x)\delta(t - t_{\text{est}})\delta(x - x_{\text{est}})\,\mathrm{d}t\,\mathrm{d}x + \int\int_\Omega C\rho\frac{\partial T}{\partial t}\Psi(t,x)\,\mathrm{d}t\,\mathrm{d}x \\ &- \int\int_\Omega \frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right)\Psi(t,x)\,\mathrm{d}t\,\mathrm{d}x + \int\int_\Omega \delta T\Psi\,\mathrm{d}t\,\mathrm{d}x. \end{aligned} \tag{7}$$

Here Ψ is the adjoint temperature; its regularity is discussed below.

Local truncation errors represented in a form of the source $\delta T(t,x)$ disturb the temperature field $\widetilde{T}$. By expanding Eq. (5a) in a Taylor series and taking first order term we obtain a problem for temperature disturbance ΔT (continuous error) assuming the form:

$$C\rho\frac{\partial\Delta T}{\partial t} - \lambda\frac{\partial^2\Delta T}{\partial x^2} + \delta T(t,x) = 0, \tag{8}$$

$$\text{Initial conditions:}\quad \Delta T(0,x)=0,$$
$$\text{Boundary conditions:}\quad \left.\frac{\partial \Delta T}{\partial x}\right|_{x=0}=0;\quad \left.\frac{\partial \Delta T}{\partial x}\right|_{x=X}=0. \tag{9}$$

We consider here $\lambda =$ Const, for $\delta T(t,x)\in C^{\infty}(Q)$, the problem is well-posed for $\Delta T(t,x)\in C^{\infty}(Q)$.

Problem (8) may be solved by using some part of Taylor expansion for sources $\delta T(t,x)$ estimation (as in [9]) that enables a correction of the target functional. Nevertheless, this is not sufficient for our purposes, since we are interested in the contribution of every grid cell to the total error and in obtaining an error bound. So we continue the analysis and calculate the variation of the Lagrangian $\Delta L(\delta T,\Psi)=L(T,\Psi)-L(\widetilde{T},\Psi)$ using Eqs. (8) and (9).

$$\Delta L(\delta T,\Psi)=\int\int_{\Omega}\Delta T\delta(t-t_{\text{est}})\delta(x-x_{\text{est}})\,\mathrm{d}t\,\mathrm{d}x+\int\int_{\Omega}\delta T\Psi\,\mathrm{d}t\,\mathrm{d}x+\int\int_{\Omega}C\rho\frac{\partial\Delta T}{\partial t}\psi\,\mathrm{d}t\,\mathrm{d}x$$
$$-\int\int_{\Omega}\frac{\partial}{\partial x}\left(\lambda\frac{\partial\Delta T}{\partial x}\right)\Psi(t,x)\,\mathrm{d}t\,\mathrm{d}x. \tag{10}$$

The formal integration of (10) by parts yields

$$\Delta L(\delta T,\Psi)=\int\int_{\Omega}\Delta T\delta(t-t_{\text{est}})\delta(x-x_{\text{est}})\,\mathrm{d}t\,\mathrm{d}x+\int\int_{\Omega}\delta T\Psi\,\mathrm{d}t\,\mathrm{d}x$$
$$-\int\int_{\Omega}C\rho\frac{\partial\Psi}{\partial t}\Delta T(t,x)\,\mathrm{d}t\,\mathrm{d}x+\int_{x}C\rho\Psi(t,x)\Delta T\,\mathrm{d}x\Big|_{t=0}^{t_f}$$
$$-\int\int_{\Omega}\frac{\partial}{\partial x}\left(\lambda\frac{\partial\Psi}{\partial x}\right)\Delta T(t,x)\,\mathrm{d}t\,\mathrm{d}x-\int_{t}\lambda\frac{\partial\Delta T}{\partial x}\Psi\,\mathrm{d}t\Big|_{x=0}^{x=X}+\int_{t}\lambda\frac{\partial\Psi}{\partial x}\Delta T\,\mathrm{d}t\Big|_{x=0}^{x=X}. \tag{11}$$

We can express the variation of the Lagrangian via the disturbing term δT

$$\Delta L=\int\int_{\Omega}\delta T\Psi(t,x)\,\mathrm{d}t\,\mathrm{d}x \tag{12}$$

if other terms in (11) are equal to zero, i.e. for the solution of following *adjoint* (*dual*) *problem*.

$$C\rho\frac{\partial\Psi}{\partial t}+\frac{\partial}{\partial x}\left(\lambda\frac{\partial\Psi}{\partial x}\right)-\delta(t-t_{\text{est}})\delta(x-x_{\text{est}})=0,\quad (t,x)\in\Omega, \tag{13}$$

$$\text{Boundary conditions:}\quad \frac{\partial\Psi}{\partial x}\Big|^{x=X}=0,\quad \frac{\partial\Psi}{\partial x}\Big|^{x=0}=0, \tag{14}$$

$$\text{Initial condition:}\quad \Psi(t_f,x)=0. \tag{15}$$

According to [5] problem (13) is well-posed for $\Psi(t,x)\in H^{-\alpha}(\Omega)$, $\frac{\alpha}{n}>\frac{1}{2}$, $\Omega\in R^{n}$. In case considered here the problem is well-posed if $\Psi(t,x)\in H^{-1}(\Omega)$, however if we smooth the source term according to [22,26], we may obtain solution $\Psi_{s}(t,x)\in H^{\beta}(\Omega)$, $\beta>1$ (although containing an error proportional to smoothing parameter $s, s>0$, which may be as small as necessary). Finite difference methods for solution of Eq. (13) are presented in [37,38,41]. The analytical solution of (13) (adjoint temperature) corresponds to a Green function of heat transfer equation [23]. For infinite space it corresponds to fundamental solution of heat transfer equation and has the following analytic form

$$\Psi(t,x)=\frac{Q}{2\sqrt{\pi\lambda/(C\rho)(t_{\text{est}}-t)}}\exp\left(-\frac{(x-x_{\text{est}})^{2}}{4\lambda/(C\rho)(t_{\text{est}}-t)}\right)\quad(\text{for } t<t_{\text{est}}).$$

It is known, [25], that $\Delta\varepsilon(\delta T) = \Delta L(\delta T, \Psi)$ for the solution of direct and adjoint problems. Thus we determine the variation of $T(t_{\text{est}}, x_{\text{est}})$.

$$\Delta\varepsilon = \Delta T_{\text{est}} = T_{\text{est}} - T_{\text{exact}} = \int\int_{\Omega} \delta T \Psi(t,x)\,\mathrm{d}t\,\mathrm{d}x. \tag{16}$$

Considering $\Psi(t,x)$ as a Green function we can conclude that expression (16) corresponds to the solution of heat conduction equation with the source δT. Hence it is bounded for bounded δT.

Thus, the adjoint temperature enables us to calculate the variation of estimated parameter as a function of the truncation error. The adjoint problem is solved in the reverse temporal direction. It is determined by the direct problem and by the choice of a checkpoint. The present statement differs from adjoint equations used in inverse heat transfer problems [4] by the form of target functional and by the form of the source in (13). Usually, problem (13) is solved by a finite-difference method, so it also contains an error $\Psi(t,x) = \Psi_{\text{exact}}(t,x) + \Delta\Psi(t,x)$. So, the error of the temperature at a checkpoint may be divided into two parts

$$\Delta\varepsilon = \Delta T_{\text{est}} = \int\int_{\Omega} \delta T \Psi_{\text{exact}}(t,x)\,\mathrm{d}t\,\mathrm{d}x + \int\int_{\Omega} \delta T \Delta\Psi(t,x)\,\mathrm{d}t\,\mathrm{d}x. \tag{17}$$

Some works [39,40] consider the minimization of the second part of expression (17) as a means for diminishing the inherent error.

3. The estimation of error caused by temporal approximation

Let us expand the mesh function T_k^n using the Taylor series with the Lagrange remainder and substitute it into finite differences (4). For the temporal part of truncation error we obtain

$$\frac{T_k^n - T_k^{n-1}}{\tau} = \frac{\partial T}{\partial t} - \frac{1}{2}\left(\tau \frac{\partial^2 T(t_n - \alpha_k^n \tau, x_k)}{\partial t^2}\right). \tag{18}$$

Parameters $\alpha_k^n \in (0,1)$ are unknown.

The last term in (18) determines δT_t, so the corresponding part of error ΔT_{est} (16) has the form

$$\Delta\varepsilon(\delta T_t) = -\frac{C\rho}{2}\int_{\Omega}\left(\tau \frac{\partial^2 T(t_n - \alpha_k^n \tau, x_k)}{\partial t^2}\right)\Psi\,\mathrm{d}x\,\mathrm{d}t. \tag{19}$$

Further discussion is mainly devoted to the calculation of magnitude and bounds of expression (19) and its analogues. Let us present (19) in a discrete form, for example:

$$\Delta\varepsilon(\delta T_t) = -\frac{C\rho}{2}\sum_{k=1,n=2}^{Nx,Nt}\left(\tau \frac{\partial^2 T(t_n - \alpha_k^n \tau, x_k)}{\partial t^2}\right)\Psi_k^n h_k \tau. \tag{20}$$

Herein N_t is a number of time steps while N_x is the number of spatial nodes.

Eq. (20) may be expanded in series over $\alpha_k^n \tau$,

$$\Delta\varepsilon(\delta T_t) = -\frac{C\rho}{2}\sum_{k=1,n=2}^{Nx,Nt}\left(\tau \frac{\partial^2 T(t_n, x_k)}{\partial t^2} - \tau\alpha_k^n \tau \frac{\partial^3 T(t_n, x_k)}{\partial t^3} + \frac{(\alpha_k^n \tau)^2}{2}\tau \frac{\partial^4 T(t_n, x_k)}{\partial t^4} - \dots\right)\Psi_k^n h_k \tau. \tag{21}$$

The first part of sum (21) may be used for correcting functional (6)

$$\Delta T_t^{\text{corr}} = -\frac{C\rho}{2}\sum_{k=1,n=2}^{Nx,Nt}\frac{\partial^2 T(t_n, x_k)}{\partial t^2}\Psi_k^n h_k \tau^2. \tag{22}$$

The second part of (21) contains unknown parameters $\alpha_k^n \in (0,1)$. If only first order term over $\alpha_k^n\tau$ is retained in (21) an upper bound may be obtained

$$\frac{C\rho}{2}\sum_{k=1,n=2}^{Nx,Nt}\alpha_k^n\tau^3\frac{\partial^3 T(t_n,x_k)}{\partial t^3}\Psi_k^n h_k \leqslant \frac{C\rho}{2}\sum_{k=1,n=2}^{Nx,Nt}\left|h_k\tau^3\frac{\partial^3 T(t_n,x_k)}{\partial t^3}\Psi_k^n\right| = \Delta T_{t,1}^{\mathrm{sup}}. \tag{23}$$

Using this value we can determine the upper bound of the functional error (after refining):

$$\left|T_{\mathrm{est}} - \Delta T_t^{\mathrm{corr}} - T_{\mathrm{exact}}\right| < \Delta T_{t,1}^{\mathrm{sup}}. \tag{24}$$

Expression (23) is the Holder inequality applied to the scalar product $(\alpha_k^n\Theta_k^n)$,

$$\sum_{k=1,n=2}^{Nx,Nt}\alpha_k^n\Theta_k^n = (\alpha_k^n\Theta_k^n) \leqslant \left\|\alpha_k^n\right\|_p\left\|\Theta_k^n\right\|_q,$$

$$\frac{1}{p}+\frac{1}{q}=1,\quad \|\alpha\|_p = (|\,\alpha_1|^p + |\,\alpha_2|^p + \cdots + |\,\alpha_N|^p)^{1/p},\quad \|\alpha\|_\infty = \max(|\,\alpha_i\,|).$$

This approach enables us to obtain estimates for other terms in (21) also. For example, the estimation of the second (over $\alpha_k^n\tau$) order term has the form

$$-\frac{C\rho}{2}\sum_{k=1,n=2}^{Nx,Nt}\left(\frac{(\alpha_k^n\tau)^2}{2}\tau\frac{\partial^4 T(t_n,x_k)}{\partial t^4}\right)\psi_k^n h_k\tau < \frac{C\rho}{2}\sum_{k=1,n=2}^{Nx,Nt}\left|\frac{1}{2}\tau^4 h_k\psi_k^n\frac{\partial^4 T(t_n,x_k)}{\partial t^4}\right| = \Delta T_{t,2}^{\mathrm{sup}}. \tag{25}$$

The estimate of the error taking into account the second term may be written as

$$|\,T_{\mathrm{est}} - \Delta T_t^{\mathrm{corr}} - T_{\mathrm{exact}}\,| < \Delta T_{t,1}^{\mathrm{sup}} + \Delta T_{t,2}^{\mathrm{sup}}. \tag{26}$$

On a sufficiently smooth solution, every next term of series $\Delta T_{t,s}^{\mathrm{sup}}$ has an order that is greater by one. For an infinitely smooth solution expression (26) may be stated as $|\,T - \Delta T_t^{\mathrm{corr}} - T_{\mathrm{exact}}\,| < \sum_{s=1}^{\infty}\Delta T_{t,s}^{\mathrm{sup}}$. If all derivatives are bounded, this series converges

$$\sum_{k=1,n=2}^{Nx,Nt}\left|\frac{(\alpha_k^n\tau)^s}{s!}\frac{\partial^{s+2}T(t_n,x_k)}{\partial t^{s+2}}\Psi_k^n h_k\tau^2\right| < C\tau\frac{\tau^s}{s!}.$$

Nevertheless, this does not guarantee the estimate to be small enough to be of practical significance.

The applicability of such estimates may be complicated by discontinuities of the derivatives. Let us consider this problem at the heuristic level. For this purpose let us write (21) in more detail.

$$\Delta\varepsilon(\delta T) = -\frac{C\rho}{2}\sum_{k=1,n=2}^{Nx,Nt}\left(\tau\frac{\partial^2 T(t_n,x_k)}{\partial t^2} - \tau\alpha_k^n\tau\frac{\partial^3 T(t_n,x_k)}{\partial t^3} + \cdots + \frac{(-\alpha_k^n\tau)^s}{s!}\tau\frac{\partial^{s+2}T(t_n,x_k)}{\partial t^{s+2}} + \cdots\right)\Psi_k^n h_k\tau. \tag{27}$$

Let m be the number of bounded derivatives (derivatives of the order m and higher may have a finite number of jump discontinuities), p is the order of the approximated derivative; j is the formal order of accuracy of a finite-difference scheme. Let us approximate derivatives by the finite differences $\frac{DT(t,x)}{Dt}$. The limit $\lim_{\tau\to 0}\sum_{\Omega}\left(\tau^j\frac{D^{p+j}T(t,x)}{Dt^{p+j}}\right)h\Psi\tau$ corresponds to the first term (27). Consider its asymptotic form. The derivative of order m+1 has an asymptotic $(T_+^{(m)} - T_-^{(m)})/\tau \sim \Delta/\tau$ for the jump discontinuity, while the derivative of order $m+2$ has the asymptotic $(\Delta/\tau - 0/\tau)/\tau \sim \Delta\ /\tau^2$, correspondingly the derivative of the order $p+j$ has the asymptotic $\frac{\Delta}{\tau^{p+j-m}}$. Thus $\lim_{\tau\to 0}\left(\tau^j\frac{D^{p+j}T(t,x)}{Dt^{p+j}}\right) \sim \lim_{\tau\to 0}\left(\tau^j\frac{\Delta}{\tau^{p+j-m}}\right)$. There are a limited number of nodes that participate in the summation in the vicinity of the discontinuity, so the multiplier τ (appearing during summation) should be taken into account, yielding $\sum_{k=1,n=n_r-n_s}^{k=Nx,n=n_r+n_s}\left(\tau^j \frac{D^{p+j}T(t,x)}{Dt^{p+j}}\right)h\Psi\tau \sim \tau^{m-p+1}$.

Thus, the terms of jth formal order of accuracy contain a component of jth order (appearing due to integration over the smooth part of the solution) and a component having the order $i = m - p + 1$ (engendered by the jump discontinuity of the mth order derivative). So, the order of convergence depends on the solution and may asymptotically tend to a minimal order $i = m - p + 1$ as grid size decreases. This is also relevant to other terms in (27).

If we have a sufficient number of smooth derivatives, we can restrict the number of terms in expansion (21) in order to avoid using derivatives of order higher than m. Let $m = 3$, then in our case ($m = j + 2$)

$$\Delta\varepsilon(\delta T) = -\frac{C\rho}{2}\sum_{k=1,n=2}^{Nx,Nt}\left(\tau\frac{\partial^2 T(t_n,x_k)}{\partial t^2} - \tau\alpha_k^n\tau\frac{\partial^3 T(t_n-\eta_k^n\alpha_k^n\tau,x_k)}{\partial t^3}\right)\Psi_k^n h_k\tau. \quad (28)$$

The derivatives in (28) are related to some points within the interval $\eta_k^n \in (0,1)$. Correspondingly, the estimation of error bound has the form

$$\Delta T_{t,1}^{\sup} = \frac{C\rho}{2}\sum_{k=1,n=2}^{Nx,Nt}\left|\tau^2\frac{\partial^3 T(t_n-\eta_k^n\alpha_k^n\tau,x_k)}{\partial t^3}\Psi_k^n\right|h_k\tau. \quad (29)$$

If the third derivative is bounded, the deviation of (29) from (23) $\left(\frac{C\rho}{2}\sum_{k=1,n=2}^{Nx,Nt}\left|\tau^2\frac{\partial^3 T(t_n,x_k)}{\partial t^3}\Psi_k^n\right|h_k\tau\right)$ is not large. Let $m = 2$, the third derivative is not bounded and the deviation of (29) from (23) may be large. In this case we should consequently estimate terms of series (27) (having the same order on τ) in the hope that the presence of the factorial $s!$ in (27) would enable us to stop summing at a certain term.

Later we will consider in numerical tests the influence of discontinuities on the error, for example that of the temperature spatial derivative.

4. Calculation of error due to spatial approximation

Similar to previous treatment we use Taylor series with a Lagrange remainder in order to estimate the discretization error of the spatial derivative. (here $\beta_k^n \in (0,1)$, $\gamma_k^n \in (0,1)$ are unknown).

$$T_{k+1}^n = T_k^n + h_k\frac{\partial T}{\partial x} + \frac{1}{2}h_k^2\frac{\partial^2 T}{\partial x^2} + \frac{1}{6}h_k^3\frac{\partial^3 T}{\partial x^3} + \frac{1}{24}h_k^4\left(\frac{\partial^4 u(t_n,x_k+\beta_k^n h_k)}{\partial x^4}\right),$$

$$T_{k-1}^n = T_k^n - h_k\frac{\partial T}{\partial x} + \frac{1}{2}h_k^2\frac{\partial^2 T}{\partial x^2} - \frac{1}{6}h_k^3\frac{\partial^3 T}{\partial x^3} + \frac{1}{24}h_k^4\left(\frac{\partial^4 u(t_n,x_k-\gamma_k^n h_k)}{\partial x^4}\right).$$

Then

$$\frac{T_{k+1}^n - 2T_k^n + T_{k-1}^n}{h_k^2} = \frac{\partial^2 T}{\partial x^2} + \frac{1}{24}h_k^2\left(\frac{\partial^4 T(t_n,x_k+\beta_k^n h)}{\partial x^4} + \frac{\partial^4 T(t_n,x_k-\gamma_k^n h)}{\partial x^4}\right). \quad (30)$$

The second part of this equation corresponds to the x-component of the disturbing term δT (δT_x) used in (16).

The error of estimated value related to the truncation error of spatial approximation has the form

$$\Delta\varepsilon(\delta T_x) = -\int_\Omega \frac{\lambda}{24}h_k^2\left(\frac{\partial^4 T(t_n,x_k+\beta_k^n h)}{\partial x^4} + \frac{\partial^4 T(t_n,x_k-\gamma_k^n h)}{\partial x^4}\right)\Psi\,dx\,dt. \quad (31)$$

Its discrete form

$$\Delta\varepsilon(\delta T_x) = -\frac{\lambda}{24}\sum_{k=1,n=1}^{Nx,Nt} h_k^2\left(\frac{\partial^4 T(t_n, x_k + \beta_k^n h)}{\partial x^4} + \frac{\partial^4 T(t_n, x_k - \gamma_k^n h)}{\partial x^4}\right)\Psi_k^n h_k \tau.$$

The first term of Taylor series expansion over $\beta_k^n h, \gamma_k^n h$ may be formulated as

$$\Delta\varepsilon(\delta T_x) = -\frac{\lambda}{12}\sum_{k=1,n=2}^{Nx,Nt} h_k^3 \frac{\partial^4 T(t_n, x_k)}{\partial x^4}\Psi_k^n \tau - \frac{\lambda}{24}\sum_{k=1,n=2}^{Nx,Nt} h_k^3\left(\frac{\partial^5 T(t_n, x_k)}{\partial x^5}\beta_k^n - \frac{\partial^5 T(t_n, x_k)}{\partial x^5}\gamma_k^n\right)\Psi_k^n h_k \tau. \tag{32}$$

The first part of this sum can be used for an error correction

$$\Delta T_x^{\mathrm{corr}} = -\frac{\lambda}{12}\sum_{k=1,n=1}^{Nx,Nt} h_k^3 \frac{\partial^4 T(t_n, x_k)}{\partial x^4}\Psi_k^n \tau. \tag{33}$$

The inherent error is engendered by the second part terms. We can obtain a bound for it by assuming $\beta_k^n - \gamma_k^n = 1$.

$$\frac{\lambda}{24}\sum_{k=1,n=2}^{Nx,Nt} h_k^3\left(\frac{\partial^5 T(t_n, x_k)}{\partial x^5}\beta_k^n - \frac{\partial^5 T(t_n, x_k)}{\partial x^5}\gamma_k^n\right)\Psi_k^n h_k \tau < \Delta T_{x,1}^{\sup} = \frac{\lambda}{24}\sum_{k=1,n=2}^{Nx,Nt} h_k^4\left|\frac{\partial^5 T(t_n, x_k)}{\partial x^5}\Psi_k^n\right|\tau. \tag{34}$$

The density in (34) $h_k^4\left|\frac{\partial^5 T(t_n,x_k)}{\partial x^5}\Psi_k^n\right|\tau$ represents the contribution of every cell to the total error, so it may serve for the design of a grid that minimizes it.

5. Numerical tests

The error is calculated for the temperature field evolution engendered by a pointwise heat source (t_0, ξ are the initial time and the coordinate of the point source).

$$T_{\mathrm{an}}(t,x) = \frac{Q}{2\sqrt{\pi\lambda/(C\rho)(t-t_0)}}\exp\left(-\frac{(x-\xi)^2}{4\lambda/(C\rho)(t-t_0)}\right), \tag{35}$$

$T_{\mathrm{an}}(t,x)$ is the analytic solution of heat conduction equation. We use the data $f_k = T_0(x_k)$ calculated by (35) as the initial data when solving (4). The length X of spatial interval is chosen so as to provide a negligible effect of the boundary condition compared with the effect of approximation. The round-off errors were estimated by comparing calculation with single and double precision, and the difference was negligible. We should also ascertain that the error $\int\int_\Omega \delta T \Delta\Psi(t,x)\,\mathrm{d}t\,\mathrm{d}x$ engendered by adjoint equation approximation is sufficiently small. For calculation of $\Delta\Psi(t,x)$ the following equation was used

$$C\rho\frac{\partial\Delta\Psi}{\partial t} + \frac{\partial}{\partial x}\left(\lambda\frac{\partial\Delta\Psi}{\partial x}\right) + \delta\Psi_t(t,x) + \delta\Psi_x(t,x) = 0 \tag{36}$$

(second order adjoint equation [2,42]). For λ = Const and $\delta T(t,x) \in C^\infty(Q)$, the problem (36) is well-posed for $\Delta\Psi(t,x) \in C^\infty(Q)$ [22].

Corresponding error of functional has the form:

$$\Delta\varepsilon(\delta T) = -\frac{C\rho}{2}\sum_{k=1,n=2}^{Nx,Nt}\left(\tau\frac{\partial^2 T(t_n, x_k)}{\partial t^2}\right)\Delta\Psi_k^n h_k \tau.$$

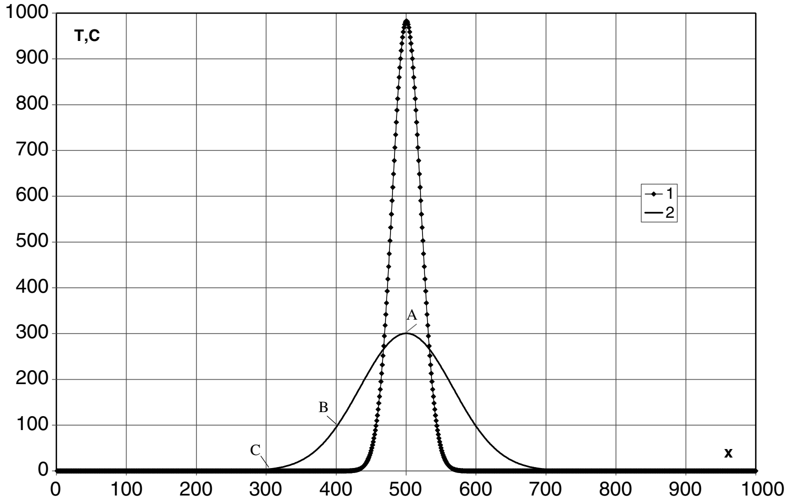

Fig. 1. Initial and final temperature distribution. (1) Initial temperature, and (2) final temperature.

As expected, numerical computations show that the part of error (17) related to the adjoint temperature error is significantly smaller than the main value (connected with the adjoint temperature itself).

An implicit method (implemented via the Thomas algorithm) was used for solution both of the heat transfer equation and the adjoint equations of first and second orders. The spatial grid consisted of 100–1000 nodes, the temporal integration contained 100–10,000 steps. Thermal conductivity was $\lambda = 10^{-4}\,\mathrm{kW/(m\,K)}$, volume heat capacity was equal to $C\rho = 500\,\mathrm{kJ/(m^3\,K)}$. The initial and final temperature distributions are presented in Fig. 1 together with zones of error estimation.

The temperature errors were estimated via adjoint equations and compared with the deviation of the numerical solution from analytical one (35).

Isolines of temperature and adjoint temperature are presented in Figs. 2 and 3 for one of computed variants.

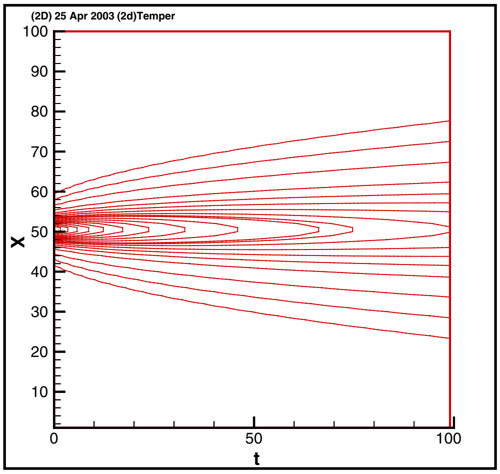

Fig. 2. Temperature isolines.

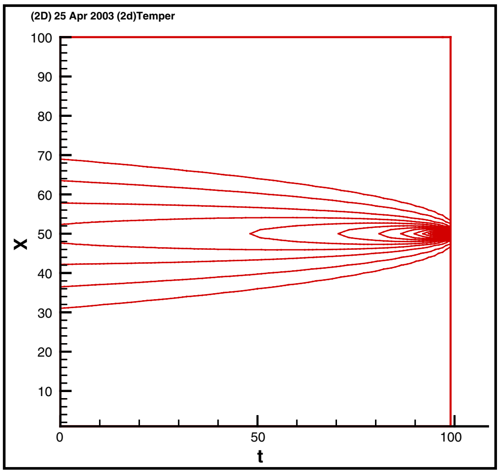

Fig. 3. Adjoint temperature isolines.

As previously mentioned, the adjoint temperature may be considered as a weight coefficient determining the contribution of the truncation error to the error of estimated parameter. Thus, Fig. 3 describes the relative weights of the truncation error contribution to the temperature at the estimated point.

6. The error caused by the truncation error of time approximation

Estimates of temperature calculation error as a function of a time step are presented in Table 1 (central point at the final moment). The spatial step is chosen to be enough small ($h = 0.0001\,\mathrm{m}$) so as to provide a small impact on the spatial discretization error in comparison with the temporal one. The error caused by adjoint temperature approximation was calculated using Eq. (36) and was significantly smaller then the temporal one.

Here $T_{\mathrm{est}} - T_{\mathrm{an}}$ is the difference between the numerical and analytical calculations, $\Delta T_t^{\mathrm{corr}}$ is the correction for the time step error, $\Delta T_x^{\mathrm{corr}}$ is the correction for the space step error, $\Delta T^{\mathrm{err}} = T_{\mathrm{est}} - \Delta T_t^{\mathrm{corr}} - \Delta T_x^{\mathrm{corr}} - T_{\mathrm{an}}$ is the deviation of refined solution from the analytical one, and $\Delta T_{t,1}^{\mathrm{sup}}$ is the upper bound of error (25) caused by the time step.

One concludes from Table 1 that the error of calculation is practically eliminated by the correction using $\Delta T_t^{\mathrm{corr}}$ and $\Delta T_x^{\mathrm{corr}}$, with the remaining part being in the range of the bound $\Delta T_{t,1}^{\mathrm{sup}}$.

We compare here ΔT^{err} and $\Delta T_{t,1}^{\mathrm{sup}}$ to illustrate that the bound is indeed satisfied.

The reader should also compare $T_{\mathrm{est}} - T_{\mathrm{an}}$ with $\Delta T_t^{\mathrm{corr}}$ to understand the quality of the correction.

Table 1
Temperature error estimations depending on the time step

τ, s	$T_{\mathrm{est}} - T_{\mathrm{an}}$	$\Delta T_t^{\mathrm{corr}}$ (23)	$\Delta T_x^{\mathrm{corr}}$ (33)	ΔT^{err}	$\Delta T_{t,1}^{\mathrm{sup}}$ (25)
0.1	0.1007	0.09301	7.75×10^{-3}	-5.0×10^{-5}	0.0113
0.2	0.1938	0.1856	7.78×10^{-3}	4.0×10^{-4}	0.0429
0.4	0.3790	0.3699	7.8×10^{-3}	1.3×10^{-3}	0.156
0.8	0.7400	0.7341	7.84×10^{-3}	-1.9×10^{-3}	0.524
1	0.9189	0.9141	7.86×10^{-3}	-3.0×10^{-3}	0.76
2	1.7904	1.7932	7.97×10^{-3}	-1.0×10^{-2}	2.15

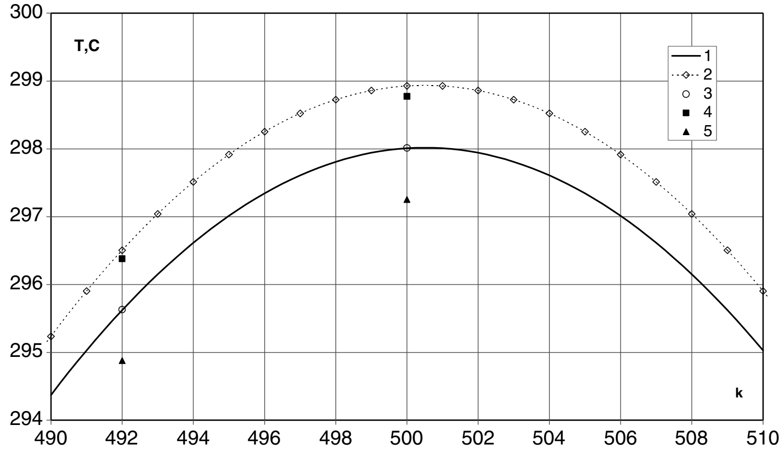

Fig. 4. The comparison between numerical and analytical solutions in zone A (Fig. 1). (1) Analytical, (2) numerical, (3) refined solution, (4) upper bound, and (5) lower bound.

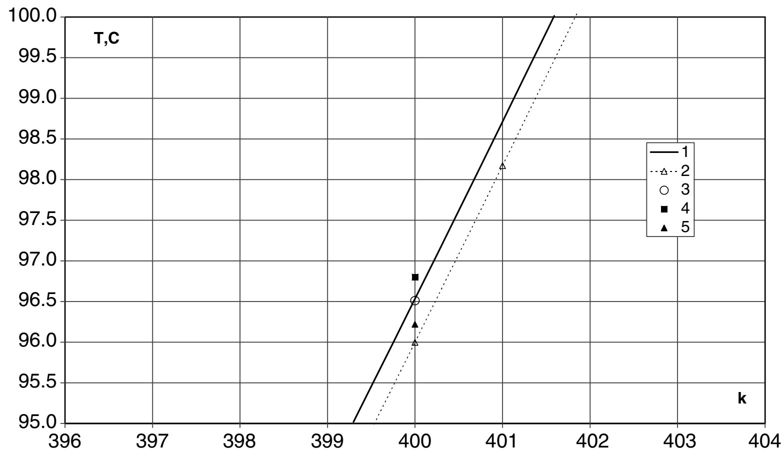

Fig. 5. The comparison between numerical and analytical solutions in zone B. (1) Analytical, (2) numerical, (3) refined solution, (4) upper bound, and (5) lower bound.

Certainly, the effectivity index [26] of bound estimation $\sim \Delta T^{\mathrm{err}}/\Delta T^{\mathrm{sup}}_{t,1}$ is rather small, nevertheless the magnitude of the upper bound is also small which ensures the practical importance of this bound.

Figs. 4–6 illustrate a comparison between analytic, finite-difference and corrected finite-difference solutions and the error bounds ($h = 0.0001\,\mathrm{m}$, $\tau = 1.0\,\mathrm{s}$) in different zones (Fig. 1).

7. The error of temperature calculation engendered by the spatial discretization

Let us consider the error caused by the truncation error of spatial approximation. In order to observe this error, let us provide a small contribution of truncation error of the temporal approximation. For this purpose a second order time approximation scheme was used.

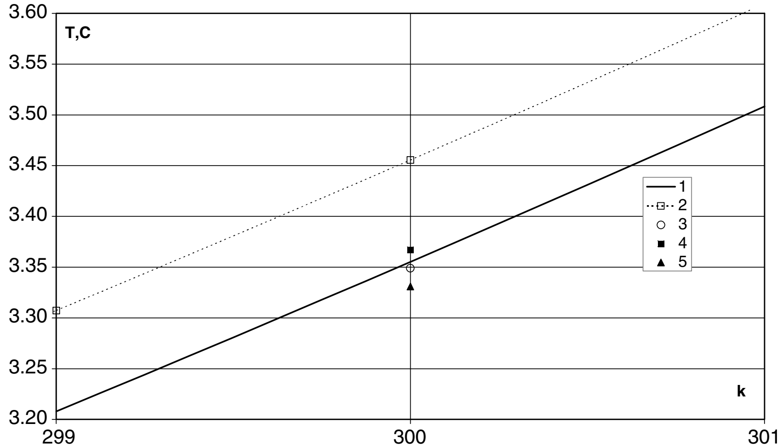

Fig. 6. The comparison between numerical and analytical solutions in zone C. (1) Analytical, (2) numerical, (3) refined solution, (4) upper bound, and (5) lower bound.

$$\begin{aligned} &C\rho\frac{T_k^{n-1/2}-T_k^{n-1}}{\tau}-\frac{1}{2}\lambda\frac{T_{k+1}^{n-1}-2T_k^{n-1}+T_{k-1}^{n-1}}{h_k^2}=0;\\ &C\rho\frac{T_k^{n}-T_k^{n-1/2}}{\tau}-\frac{1}{2}\lambda\frac{T_{k+1}^{n}-2T_k^{n}+T_{k-1}^{n}}{h_k^2}=0. \end{aligned} \tag{37}$$

It may be shown in a similar fashion as in previous treatments that the error caused by the temporal approximation is of second order in τ.

$$\Delta\varepsilon(\delta T_t)=-\frac{C\rho}{12}\sum_{k=1,n=2}^{Nx,Nt}\frac{\partial^3 T(t_n,x_k)}{\partial t^3}\Psi_k^n h_k\tau^3. \tag{38}$$

A bound on the inherent error caused by temporal step is:

$$\Delta T_t^{\sup}=\Delta\varepsilon(\delta T)=\frac{C\rho}{4}\sum_{k=1,n=2}^{Nx,Nt}\left|\frac{\partial^4 T(t_n,x_k)}{\partial t^4}\Psi_k^n\right|h_k\tau^4. \tag{39}$$

The error caused by the spatial approximation preserves its previous form (33) and (34).

Numerical tests demonstrated that the error caused by the time step (38) was not greater than 2×10^{-5} and was significantly smaller than the error caused by the spatial approximation. The error caused by the adjoint equation approximation $\int\int_\Omega \delta T\Delta\Psi(x,t)\mathrm{d}t\,\mathrm{d}x$ was still smaller by several orders of magnitude. The temperature error estimates as a function of the spatial step size are presented in Table 2 (for central point at the final time).

Table 2
Temperature error estimates depending on the spatial step

H, m	$T_{est}-T_{an}$	ΔT_x^{corr} (33)	$T_x^{corr}-T_{an}$	$\Delta T_{x,1}^{sup}$ (34)
0.002	3.0607	2.719	0.341	6.3
0.001	0.772345	0.751934	0.0204	1.86
0.0008	0.494818	0.48683	0.0080	1.08
0.0004	0.123853	0.123579	2.74×10^{-4}	0.163
0.0002	0.030948	0.031011	6.3×10^{-6}	2.1×10^{-2}
0.0001	0.007711	0.007760	4.9×10^{-5}	2.7×10^{-3}

The comparison of deviations of solution and refined solution ($T_x^{\rm corr} = T_{\rm est} - \Delta T_x^{\rm corr}$) from analytical one ($T_{\rm est} - T_{\rm an}$ and $T_x^{\rm corr} - T_{\rm an}$) demonstrates that the refinement by $\Delta T_x^{\rm corr}$ (33) enables us to eliminate a significant part of the error. Comparison of the remaining error $T_x^{\rm corr} - T_{\rm an}$ and $\Delta T_{x,1}^{\rm sup}$ shows a reliable satisfaction of the bound (34). The remaining error $T_x^{\rm corr} - T_{\rm an}$ contains all uncontrolled errors including those caused by boundary terms, errors of upper orders etc., so it has a rather irregular behavior.

The quadratic character of $\Delta T_x^{\rm corr}$ and the third order of $\Delta T_x^{\rm sup}$ should be noted. The convergence rate of $\Delta T_x^{\rm corr}$ and $\Delta T_x^{\rm sup}$ demonstrates that discontinuities of high order derivatives for Eq. (1) under initial conditions (35) and boundary conditions (2) did not engender any visible effect (they are located in zones of small Ψ).

Fig. 7 illustrates the initial and final temperature distributions ($h = 0.001$ m, $\tau = 0.1$ s). Figs. 8 and 9 provide a comparison between the analytical, finite-difference and refined solutions and the error bound at different points (zones A and B, Fig. 7). The spatial step is chosen large enough for visibility and for suppression of other errors. As expected, the error is smaller for finer mesh (Table 2).

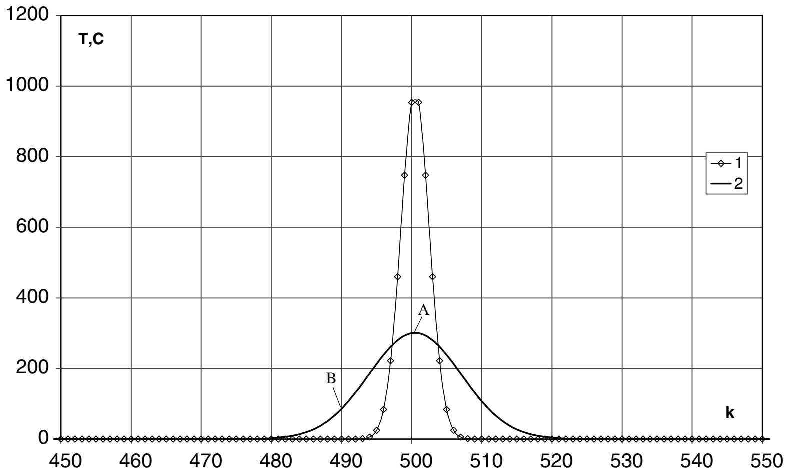

Fig. 7. Initial and final temperature distribution. (1) Initial temperature, and (2) final temperature.

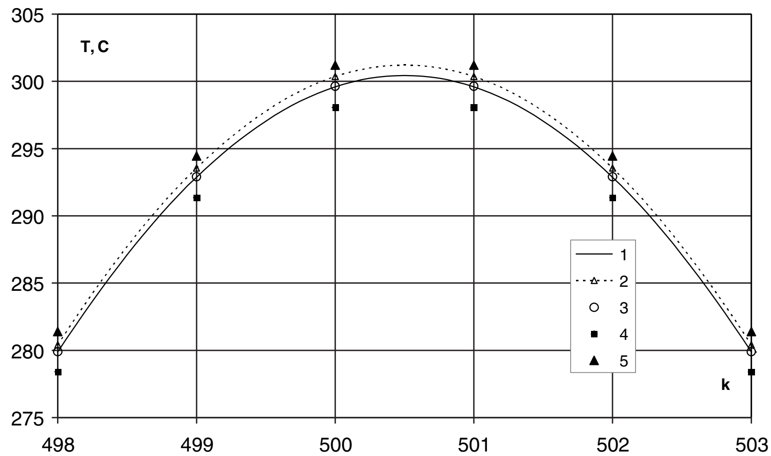

Fig. 8. The refined solution and error bounds in comparison with finite-difference and analytical solution. Zone A (Fig. 7). (1) Analytical, (2) numerical, (3) refined solution, (4) lower bound, and (5) upper bound.

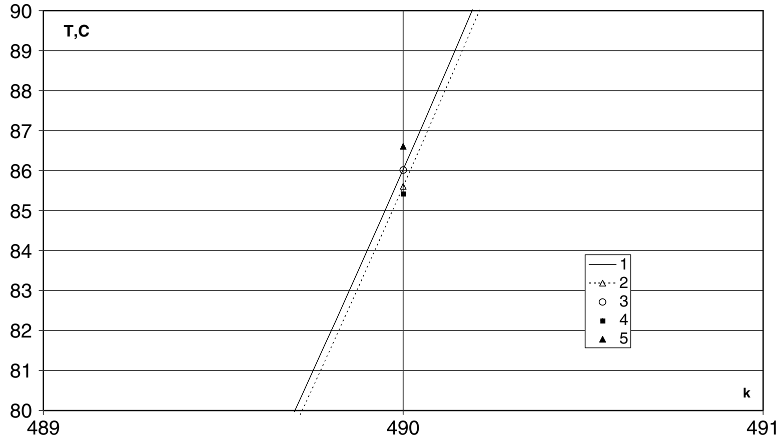

Fig. 9. The refined solution and error bounds in comparison with finite-difference and analytical solution. Zone B (Fig. 7). (1) Analytical, (2) numerical, (3) refined solution, (4) lower bound, and (5) upper bound.

8. Influence of discontinuities

A calculation of ΔT_x^{corr} and ΔT_x^{sup} requires bounded high order derivatives. These are not always available, nevertheless (as already shown), the limitations on the smoothness requirements may be slightly relaxed. If the corresponding derivatives of the exact solution have jump discontinuities, $(\widetilde{T} \in H^2_{\text{loc}}(\Omega))$ the integral estimates of error exist, but asymptotically reveal existence of another (smaller) order of convergence. Hence, the thermal conductivity stepwise discontinuities (engendering discontinuities of temperature gradient) are potential sources of errors, which may be significantly greater than the nominal error of the finite-difference scheme. Herein we focus our attention on the discontinuities of primal parameters. The adjoint parameters are not differentiated, so are not so dangerous for our calculations. Some information on discontinuities of primal and adjoint parameters in related problems may be found in [12,14,19].

Let us carry out numerical tests to study the asymptotic dependence of the error on the space step size for a temperature gradient discontinuity. In order to deal with the discontinuity we used a divergent integro-interpolation method [35] assuming the following form:

First step

$$C_k\rho_k\frac{T_k^{n+1/2}-T_k^n}{\tau} = Z_{k+1/2}\left(T_k^n - T_{k+1}^n\right) + Z_{k-1/2}\left(T_k^n - T_{k-1}^n\right). \tag{40a}$$

Second step

$$C_k\rho_k\frac{T_k^{n+1}-T_k^{n+1/2}}{\tau} = Z_{k+1/2}\left(T_k^{n+1} - T_{k+1}^{n+1}\right) + Z_{k-1/2}\left(T_k^{n+1} - T_{k-1}^{n+1}\right), \tag{40b}$$

where

$$Z_{k+1/2} = \frac{2}{h_k\left(\dfrac{h_k}{\lambda_k}+\dfrac{h_{k+1}}{\lambda_{k+1}}\right)}; \quad Z_{k-1/2} = \frac{2}{h_k\left(\dfrac{h_k}{\lambda_k}+\dfrac{h_{k-1}}{\lambda_{k-1}}\right)}.$$

Corresponding estimates of the form (33) and (34) may be easily deduced but are very bulky and are not presented here. They may be found in [3].

Table 3
Temperature error estimates as a function of the spatial step

h, m	ΔT_x^{corr}	$\Delta T_{x,1}^{\text{sup}}$	$\Delta T_{x,2}^{\text{sup}}$	$\Delta T_{x,3}^{\text{sup}}$	$\Delta T_{x,4}^{\text{sup}}$
0.0016	4.6×10^{-1}	2.7	2.45	6.9×10^{-1}	1.6×10^{-1}
0.0008	3.02×10^{-1}	8.61×10^{-1}	5.59×10^{-1}	1.28×10^{-1}	2.48×10^{-2}
0.0004	9.39×10^{-2}	4.1×10^{-1}	3.89×10^{-1}	1.19×10^{-1}	2.92×10^{-2}
0.0002	2.77×10^{-2}	3.57×10^{-1}	4.13×10^{-1}	1.32×10^{-1}	3.26×10^{-2}
0.0001	7.32×10^{-3}	2.24×10^{-1}	2.63×10^{-1}	8.58×10^{-2}	2.09×10^{-2}
0.00005	1.84×10^{-3}	1.2×10^{-1}	1.42×10^{-1}	4.65×10^{-2}	1.13×10^{-2}

Table 3 presents temperature error estimates (for central point at the final moment) depending on the spatial step for the thermal conductivity coefficient having a 10% jump at the center of the grid.

The data of Table 3 shows that ΔT_x^{corr} has a convergence order similar to the smooth case (Table 2), while $\Delta T_{x,s}^{\text{sup}}$ has a low order (not higher than one) and decreases relatively slowly when the number of terms increases. This difference in behavior is caused by the compensation of the error before and past the stepwise discontinuity in the expression for ΔT_x^{corr} (33). Similar effects are well known in CFD ([21], for example). Corresponding expressions for $\Delta T_{x,s}^{\text{sup}}$ contain moduli, so a compensation of the error before and past the discontinuity is impossible.

As another test we consider the evolution of the initial temperature distribution of a step shape. The initial, the final distribution of temperature, and the location of estimated points are presented in Fig. 10. The stepwise discontinuity of thermal conductivity is located at center point ($x_s = X/2$) and coincides with a stepwise discontinuity of the initial temperature.

On the left part of Fig. 10, the initial temperature is denoted as T_{01}, thermophysical parameters are marked by index 1, correspondingly. On the right part of Fig. 10 the initial temperature is marked as T_{02}, while thermophysical parameters are marked by index 2, and the value of thermal conductivity is doubled comparing the left part. The thermal conductivity stepwise discontinuity causes a discontinuity in the temperature derivative which is of special interest here.

The corresponding analytical unsteady solution is described by expressions

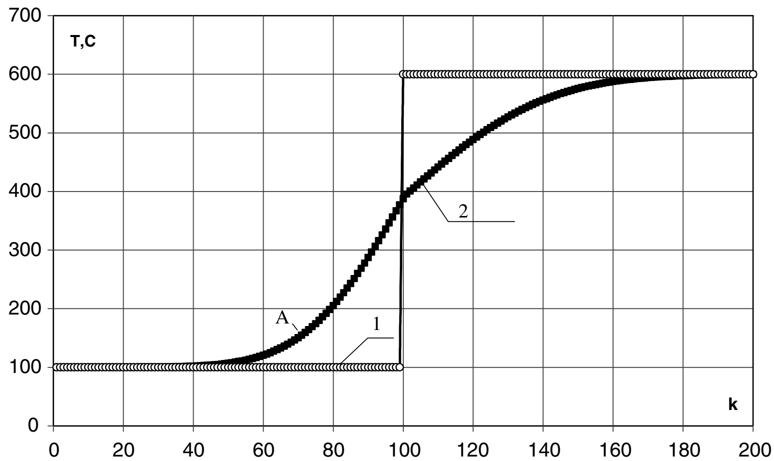

Fig. 10. Initial and final temperature distribution. (1) Initial temperature, and (2) final temperature, A—zone of estimation.

Table 4
Estimates of temperature error in dependence on spatial step

h, m	$T_{est} - T_{an}$	ΔT_x^{corr}	$\Delta T_{x,1}^{sup}$	$\Delta T_{x,2}^{sup}$	$\Delta T_{x,3}^{sup}$	$\Delta T_{x,4}^{sup}$
0.0016	-4.0×10^{-1}	-3.7×10^{-1}	8.9×10^{-1}	1.15	3.7×10^{-1}	9.2×10^{-2}
0.0008	-1.55×10^{-1}	-1.4×10^{-1}	5.5×10^{-1}	6.6×10^{-1}	2.13×10^{-1}	5.3×10^{-2}
0.0004	-5.0×10^{-2}	-5.3×10^{-2}	3.6×10^{-1}	4.3×10^{-1}	1.4×10^{-1}	3.4×10^{-2}
0.0002	-1.2×10^{-2}	-2.0×10^{-2}	2.7×10^{-1}	3.3×10^{-1}	1.02×10^{-1}	2.6×10^{-2}

$$\frac{T_{an}(t,x) - T_{01}}{T_{02} - T_{01}} = \frac{\theta}{1+\theta}(1 - \operatorname{erf}(-U_1)), \quad x < x_s, \tag{41}$$

$$\frac{T_{an}(t,x) - T_{01}}{T_{02} - T_{01}} = \frac{\theta}{1+\theta}\left(1 + \frac{\operatorname{erf}(U_2)}{\theta}\right), \quad x > x_s, \tag{42}$$

$$\theta = \left(\frac{\lambda_2 C_2 \rho_2}{\lambda_1 C_1 \rho_1}\right)^{0.5}, \quad U_i = \frac{x - x_s}{2\sqrt{\lambda_i/(C_i\rho_i)t}}, \quad \operatorname{erf}(U_i) = \frac{2}{\sqrt{\pi}}\int_0^{U_i} e^{-u^2}\,du. \tag{43}$$

The deviation of finite-difference calculation from the analytical value and estimates of the errors are presented in Table 4.

The rate of convergence of $T_{est} - T_{an}$ and ΔT_x^{corr} is close to second order despite the influence of discontinuity. This is caused by mutual compensation of error in the vicinity of discontinuity as confirmed by an analysis of local distribution of error density $-\frac{\lambda}{12} h_k^3 \frac{\partial^4 T(t_n,x_k)}{\partial x^4} \Psi_k^n \tau$ (engendering ΔT_x^{corr} in accordance with (33)). The order of $\Delta T_{x,s}^{sup}$ is close to one (slightly below), which corresponds to the expected influence of the temperature gradient discontinuity. Calculations show the upper bound of error $\Delta T_{x,1}^{sup}$ to be quite reliable; hence computation of the next terms is rendered unnecessary.

Thus, refining of the finite-difference solution and calculation of error bound using adjoint temperature may also be performed in presence of discontinuities in the temperature gradient.

9. Discussion

The approach considered above is limited by the need to use temperature derivatives of high order that may be unbounded. In the first test problem, we used initial data $f_k = T_0(x_k)$ that are calculated analytically (35). The problem (1) with these initial data (on infinite space interval) provides existence of an infinite number of temporal and spatial derivatives. Here we use a finite spatial interval X and boundary conditions (2), so the discontinuities on the boundaries are unavoidable. Nevertheless, for the time duration considered in the paper the adjoint temperature is close to zero near the boundary. This allows applicability of estimates using high order derivatives.

For the solution, having m bounded derivatives, we can obtain a correction and upper bound for the finite-difference approximation of the pth derivative under condition that $m - p \geqslant 0$. Nevertheless, for small number of bounded derivatives ($m = p$) refinement does not increase the convergence rate (correcting and upper bound terms have the same order). Even after refinement, the error still contains a component of first order, and the upper bound (28) may contain an indefinite number of terms and may be too large. For a smoother solution ($m - p \geqslant 1$), it is feasible to raise the minimal convergence order by one and obtain an upper bound of error using a single term of next higher order. And only for a smooth enough solution ($m \geqslant j + p + 1$, j-approximation order) is it feasible to raise the nominal order of scheme accuracy and obtain upper bounds of next order of accuracy.

Naturally, the present approach enables us to compute not only the error of temperature (written in the form of functional (6)) but also the error of other functionals of temperature. The differences are only in the form of the source in the adjoint equation (13).

10. Conclusion

The numerical tests presented in this paper demonstrate that the pointwise error of finite-difference solution of heat conduction equation may be reduced using differential approximation of finite difference scheme in conjunction with the adjoint equation.

The bound on the remaining error may be obtained as a function of the sizes of temporal and spatial steps.

As shown by numerical tests, the first upper bound estimate is reliable enough for smooth solutions. As the mesh size is reduced, numerical tests exhibit a convergence rate higher by one than the order of the finite difference scheme. Even in the presence of discontinuities in the temperature gradients, numerical computations demonstrated the possibility of obtaining realistic upper bounds despite a reduction in the convergence order.

This approach may be used for calculation of other quantities of interest (temperature functionals) with preset levels of accuracy or for the design of an optimal mesh. The computer time required for the refining and for the bound calculation is equal to the CPU time required for temperature computation on a mesh of similar size.

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