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CALCULATION OF A TEMPERATURE ERROR BY THE CONJUGATE EQUATION

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A temperature error depending on the error of initial information can be calculated by the conjugate problem. On estimation of the error at one time- and coordinate-local point the expenditures of the computation time and computer memory are double the expenditures for calculation of the heat-conduction equation. The conjugate-temperature field obtained in this case allows calculation of the effect of the error of any parameter of the problem (initial conditions, boundary conditions, coefficients). In the linear case, the conjugate-temperature field depends on the position of the point under estimation; in the nonlinear case, it additionally depends on the temperature field. The approach considered can be applied to calculation of the error of a wide class of temperature functionals.

Introduction. A temperature error can be found from the error of the initial data using the sensitivity equations, Monte Carlo methods, or conjugate equations of second kind. However, all these approaches are characterized by high requirements on the high-speed operation and memory; therefore, in practice, algorithms which evaluate the error of computational results are few and far between.

In what follows, the conjugate equations which are close to the equations used in solution of inverse problems of heat conduction are employed for estimation of the error of the initial data [1]. This approach to local (at a certain control point over the coordinate and time) estimation of accuracy is ultimately economical from the point of view of calculation, since only one conjugate equation must be solved in addition to the heat-conduction equation. The "conjugate temperature" obtained as a result allows one to calculate the the effect of error of all parameters of the equation.

Estimation of the Calculation Error. We consider the scheme of estimation of the error with an example of solution of a one-dimensional equation of heat conduction:

$$C\rho \frac{\partial T}{\partial t} - \frac{\partial}{\partial X}\left(\lambda (T) \frac{\partial T}{\partial X}\right) = 0 ; \quad (t, X) \in (0 < t < t_k ; \quad 0 < X < 1) . \tag{1}$$

The initial conditions are

$$T (0, X) = T_0 (X) . \tag{2}$$

The heat flux $Q_w(t)$ is operative on one boundary:

$$\lambda \frac{\partial T}{\partial X}\bigg|_{X=1} = Q_w (t) , \tag{3}$$

and the other boundary is thermally insulated:

$$\frac{\partial T}{\partial X}\bigg|_{X=0} = 0 . \tag{4}$$

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We assume that the heat flux on one boundary $Q_w(t)$, the initial temperature $T_0(X)$, and the coefficient of thermal conductivity written as $\lambda = \lambda_0 f(T)$ have an error. Below, for the sake of brevity, we simultaneously use the notations λ and $\lambda_0 f(T)$.

Let discrete representations of the parameters $Q_w(t)$, $T_0(X)$, and λ_0 have an independent normally distributed error. It is necessary to calculate the temperature error at a certain control point $T(t_{est}, x_{est})$, namely, the dispersion of the temperature depending on the dispersion of the initial data $\sigma_T^2 = f(\sigma_Q^2, \sigma_{T_0}^2, \sigma_{\lambda_0}^2)$ at the point $T(t_{est}, x_{est})$.

We denote $T(t_{est}, x_{est})$ as $\varepsilon(Q_w(t), T_0(x), \lambda_0)$ and write as a functional

$$\varepsilon\,(Q_w\,(t)\,,\,T_0\,,\,\lambda_0) = \iint\limits_{\Omega} T\,(t,\,x)\,\delta\,(t - t_{est})\,\delta\,(x - x_{est})\,dtdx\,. \tag{5}$$

In the case of the normally distributed statistical independent error of the data, the dispersion of the result can be calculated in terms of the dispersion of the error of the initial data and the value of the corresponding gradient [2]; in the case considered,

$$\sigma_\varepsilon^2 = \sum_{i=1}^{N_t} \left(\frac{\partial \varepsilon}{\partial Q_i}\,\sigma_{Q_i}\right)^2 + \sum_{j=1}^{N_x} \left(\frac{\partial \varepsilon}{\partial T_i}\,\sigma_{T_i}\right)^2 + \left(\frac{\partial \varepsilon}{\partial \lambda_0}\,\sigma_{\lambda_0}\right)^2. \tag{6}$$

It is known that the most effective method of calculation of the gradient is based on use of the conjugate equation [1, 3]; it makes sense to use this approach here. However, the conjugate equation employed in this work somewhat differs from the standard form used in inverse problems [1]. We consider the derivation of it. To do this, we introduce the Lagrangian $L(Q_w, T_0, \lambda_0, \Psi)$, which consists of the estimated quantity and ill-posed of problem (1):

$$L\,(Q_w\,(t)\,,\,T_0\,,\,\lambda_0,\,\Psi) = \iint\limits_{\Omega} T\,(t,\,x)\,\delta\,(t - t_{est})\,\delta\,(x - x_{est})\,dtdx +$$

$$+ \iint\limits_{\Omega} \rho C\,\frac{\partial T}{\partial t}\,\Psi\,(x,\,t)\,dtdx - \iint\limits_{\Omega} \frac{\partial}{\partial X}\left(\lambda_0 f\,(T)\,\frac{\partial T}{\partial X}\right)\Psi\,(x,\,t)\,dtdx\,. \tag{7}$$

We consider the effect of variation of the boundary conditions ΔQ_w, initial conditions $\Delta T_0(X)$, and the coefficient $\Delta\lambda_0$, which disturbs the temperature field. Having subtracted a nondisturbed solution, we obtain the problem

$$C\rho\,\frac{\partial \Delta T}{\partial t} - \frac{\partial}{\partial X}\left(\lambda\,\frac{\partial \Delta T}{\partial X} + \Delta\lambda_0 f\,(T)\,\frac{\partial T}{\partial X} + \lambda_0\,\frac{\partial T}{\partial X}\,\frac{\partial f}{\partial T}\,\Delta T\right) = 0\,. \tag{8}$$

The initial conditions are

$$\Delta T\,(0,\,X\,) = \Delta T_0\,(X\,)\,, \tag{9}$$

the boundary conditions are

$$\left.\frac{\partial \Delta T}{\partial X}\right|_{X=0} = 0\,; \quad \lambda\,\left.\frac{\partial \Delta T}{\partial X}\right|_{X=1} = \Delta Q_w\,(t)\,. \tag{10}$$

Then, Eqs. (8)–(10) are used to calculate the variation of Lagrangian (7)

$$\Delta L\,(Q_w\,(t)\,,\,T_0\,(x)\,,\,\lambda_0) = \iint\limits_{\Omega} \Delta T\delta\,(t - t_{est})\,\delta\,(x - x_{est})\,dtdx +$$

$$+ \iint\limits_{\Omega} \rho C\,\frac{\partial \Delta T}{\partial t}\,\Psi\,dtdx - \iint\limits_{\Omega} \frac{\partial}{\partial X}\left(\lambda\,\frac{\partial \Delta T}{\partial X} + \Delta\lambda_0 f\,(T)\,\frac{\partial T}{\partial X} + \lambda_0\,\frac{\partial T}{\partial X}\,\frac{\partial f}{\partial T}\,\Delta T\right)\Psi\,(x,\,t)\,dtdx\,. \tag{11}$$

Integration of Eq. (11) by parts yields

$$\Delta L\,(Q_{\rm w}\,(t)\,,\,T_0\,(x)\,,\,\lambda_0) = \iint\limits_{\Omega} \Delta T\delta\,(t-t_{\rm est})\,\delta\,(x-x_{\rm est})\,dtdx - \iint\limits_{\Omega} \rho C\,\frac{\partial\Psi}{\partial t}\,\Delta T\,(x,\,t)\,dtdx + \int\limits_{X} \rho C\Psi\,(X,\,t)\,\Delta T dX\,\Big|_{t=0}^{t=1} -$$

$$-\,\Delta\lambda_0 \iint\limits_{\Omega} \frac{\partial}{\partial X}\left(f\,(T)\,\frac{\partial T}{\partial X}\right)\Psi\,dtdx + \lambda_0 \iint\limits_{\Omega} \frac{\partial\Psi}{\partial X}\,\frac{\partial T}{\partial X}\,\frac{\partial f}{\partial T}\,\Delta T\,dtdx - \lambda_0 \int\limits_{t} \frac{\partial T}{\partial X}\,\frac{\partial f}{\partial T}\,\Delta T\Psi\,dt\,\Big|_{x=0}^{x=1} -$$

$$-\iint\limits_{\Omega} \frac{\partial}{\partial X}\left(\lambda\,\frac{\partial\Psi}{\partial X}\right)\Delta T\,(x,\,t)\,dtdx - \int\limits_{t} \lambda\,\frac{\partial\Delta T}{\partial x}\,\Psi dt\,\Big|_{x=0}^{x=1} + \int\limits_{t} \lambda\,\frac{\partial\Psi}{\partial x}\,\Delta T dt\,\Big|_{x=0}^{x=1}. \qquad (12)$$

Hence we can estimate variation of the Lagrangian in terms of variations of the parameters containing the error:

$$\Delta L = -\int\limits_{t} \lambda\,\frac{\partial\Delta T}{\partial X}\,\Psi\,(t,\,1)\,dt - \rho C \int\limits_{X} \Delta T\,\Psi\,(0,\,x)\,dx - \Delta\lambda_0 \iint\limits_{\Omega} \frac{\partial}{\partial X}\left(f\,(T)\,\frac{\partial T}{\partial X}\right)\Psi\,dtdx\,. \qquad (13)$$

Conjugate Problem. Expression (13) holds if all the remaining terms in (12) are zero. The corresponding conditions have the form of the problem

$$\rho C\,\frac{\partial\Psi}{\partial t} + \lambda\,\frac{\partial^2\Psi}{\partial X^2} - \lambda_0\,\frac{\partial\Psi}{\partial X}\,\frac{\partial T}{\partial X}\,\frac{\partial f}{\partial T} - \delta\,(t-t_{\rm est})\,\delta\,(x-x_{\rm est}) = 0\,, \qquad (14)$$

the boundary conditions are

$$\lambda\,\frac{\partial\Psi}{\partial X}\bigg|^{X=1} = 0\,, \quad \lambda\,\frac{\partial\Psi}{\partial X}\bigg|^{X=0} = 0\,, \qquad (15)$$

the initial condition is

$$\rho C\,\Psi\,(t,\,x)\,\big|^{t=1} = 0\,. \qquad (16)$$

It can be shown that in solution of (14)–(16), $\Delta L(Q_{\rm w}(t),\,T_0(x),\,\lambda_0) = \Delta\varepsilon(Q_{\rm w}(t),\,T_0(x),\,\lambda_0)$, which allows calculation of the gradient of the objective functional. Formulation (14)–(16) differs from the conjugate equations used in the inverse problems of heat conduction [1] in the form of the objective functional and, correspondingly, in the form of the source in (14). The conjugate problem is solved in the opposite direction over time. It is determined by the direct problem and the choice of the measurement point and does not depend on the choice of the parameter, the effect of whose error we estimate. Therefore, the same conjugate-temperature field can be used for calculation of the propagation of errors of different parameters. Conjugate temperature allows calculation of the gradient of the estimated parameter and, correspondingly, transfer of error (6):

$$\nabla\varepsilon_Q = -\,\Psi\,(t,\,1)\,, \quad \nabla\varepsilon_{T_0} = -\,\rho C\,\Psi\,(0,\,x)\,, \quad \nabla\varepsilon_{\lambda_0} = -\iint\limits_{\Omega} \frac{\partial}{\partial x}\left(\frac{\partial T}{\partial X}\,f\,(T)\right)\Psi\,dtdx\,. \qquad (17)$$

The calculation of the gradient requires successive solution of the direct and conjugate problems. Thus, the time spent for calculation of the error at one point is approximately equal to two times the solution of the heat-conduction problem. In the linear case, the third term in Eq. (14) disappears, the conjugate problem does not depend on the temperature field, and the field of conjugate parameters can be calculated once for all cases.

Results of Test Calculations. By way of illustration, we calculated the temperature error on the inner surface of a plate (thickness 3 mm) at a finite instant of time. The heat flux affecting the outer surface was taken as the parameter which involves an error. The problem had 20 cells over the thickness and 28 heat-flux nodes over time (with

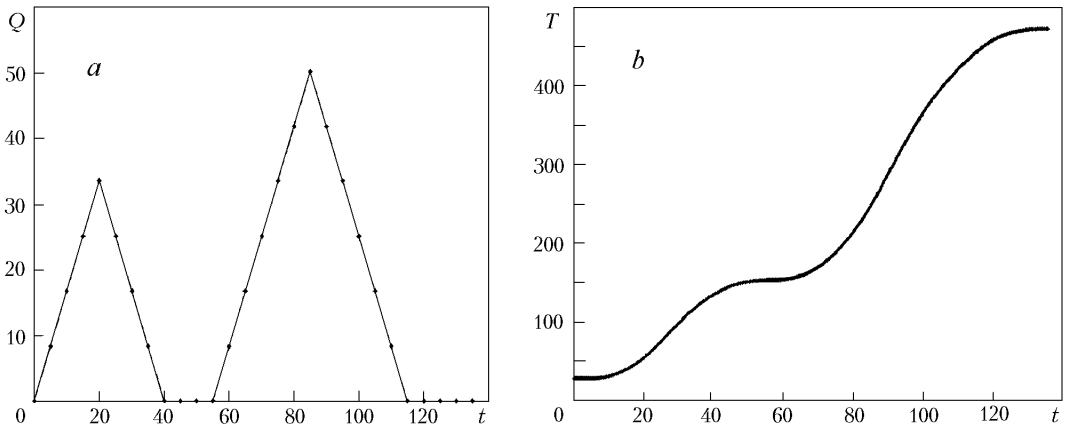

Fig. 1. Temperature mode of the test problem: a) heat flux to the heated surface; b) temperature at the measurement point.

an interval of 5 sec). The thermal conductivity of the material is $\lambda = 10^{-4}$ kW/(m·sec·K) and the bulk heat capacity is $C\rho$ = 500 kJ/(m^3·K). The surface heat flux and the temperature at the measurement point are shown in Fig. 1 (the thermal mode is similar to that described in [4]).

To solve both the heat-conduction equation and the conjugate equation we used the integro-interpolation method. In this case, the singular source in (14) is integrated with respect to the cell and gives a source of the type $\delta_{ij}/(\Delta t \Delta X)$ (δ_{ij} is the Kronecker symbol). This expression is potentially dangerous from the point of view of numerical realization, since its value decreases with an increase in the grid mesh. There were no difficulties in our calculations, but in other cases this expression would have to be approximated by a certain smooth curve, e.g., the Gauss distribution.

The standard deviation of the temperature error at a finite instant of time on the inner surface was calculated by the conjugate temperature and the Monte Carlo method for a normally distributed heat-flux error with a standard deviation of 0.4 kW/m^2. The standard deviation of the temperature error calculated by the conjugate temperature is 3.72^{o}C, whereas the calculation of this quantity by the Monte Carlo method (averaging over 200 calculations) gave a value of 3.32^{o}C. Although the results are close, the ratio of the times of calculation is 100 times. For large-scale problems (for example, three-dimensional ones) this ratio of the calculation times can justify writing of the conjugation code.

Discussion. We consider the computational efficiency of different approaches to calculation of the error.

The dispersion of temperature within the entire computational field can be found by the coefficients of sensitivity, for example, $S(t, x, \tau) = \partial t(T, x)/\partial Q(\tau)$, $\langle \delta T^2(x, t) \rangle = S_k \langle dQ_k dQ_l \rangle S_l$. The sensitivity function satisfies the equations

$$\rho C \frac{\partial S}{\partial t} + \lambda \frac{\partial^2 S}{\partial X^2} = 0 , \tag{18}$$

The boundary conditions are

$$\lambda \frac{\partial S}{\partial X}\bigg|_{X=1} = \delta (t - \tau) , \quad \lambda \frac{\partial S}{\partial X}\bigg|_{X=0} = 0 , \tag{19}$$

the initial condition is

$$S (t = 0) = 0 . \tag{20}$$

This method implies the solution of a higher-order system (the dimensionality of the parameters involving the error) compared to problem (1)–(4) and the storage of multi-dimensional results of calculations. In our case, the calcu-

lation of sensitivity corresponds to N_t calculations of the direct problem. To find the total field of the error by conjugate equations, we need $N_x N_t + 1$ calculations. Thus, if it is necessary to know the error distribution within the entire computational field, the sensitivity equations provide more efficient calculation compared to the use of the conjugate equations.

In comparison of the methods of calculation of the sensitivity equations (18)–(20) and the method under consideration, one should allow for the fact that the calculation of conjugate equations is perfectly suited to the use of parallel computers of the cluster type. The calculation of errors of N parameters requires solution of N identical independent problems of the calculation of conjugate equations (14)–(16) which differ only in the position of the source. Unparallelization of the system (18)–(20) is a much more complex problem, which causes a loss of efficiency with increase in the number of processors.

The Monte Carlo methods are rather expensive from the point of view of the time of calculation and, if the coefficients of sensitivity are unknown, they give only asymptotically accurate results. This is due to the fact that the error of the result, depending on the number of tests, decreases as $c(N, S)/M^{0.5}$, where $c(N, S)$ is a constant which depends only on the number N of parameters involving an error and on the coefficients of sensitivity S. However, the Monte Carlo methods can be realized in a simpler way from an algorithmic standpoint. They do not require solution of auxiliary problems and can be competitive at sufficient computational powers.

In some problems, the contribution of the gradient in the expression for variation of the objective functional $\delta\varepsilon = \nabla\varepsilon_{ki}\delta U_k + 0.5H_{kl}\delta U_k\delta U_l$ can be small compared with the contribution of the Hessian. For example, as a measure of the error we can take the mean deviation of the temperature over a certain region or time interval [4]. For time-averaging, the objective functional has the form

$$\varepsilon\left(\delta Q_{\mathrm{w}}(t)\right) = \int_t \left(T_{X=0}(t) - T^{\mathrm{err}}_{X=0}(t)\right)^2 dt\,.$$

This functional corresponds to the discrepancy between accurate and noisy solutions. In such a formulation the problem is solved by second-order conjugate equations [4, 5]. This approach is based on calculation of the Hessian (or a part of its spectrum) and, in the general case, requires expenditures of the computation time which are proportional to the number of parameters involving an error. It is worth employing the method of [4] for estimation of the accuracy of the functionals near the extremum points. For calculation of the error at one point this method ranks below the approach under consideration in expenditure of resources and the complexity of the algorithm.

As a whole, if we are interested in an error at a certain point, the conjugate equations in the form considered in the paper are the most efficient relative to the time of computation and the volume of results stored. They are also very promising from the point of view of calculation of an error of a large massif of points (for example, calculation of an error of the time-dependence of temperature in a set of control points) in the use of parallel computers.

Needless to say, this approach allows calculation of both an error of the temperature written in the form of functional (5) and the error of other temperature functionals, and also a number of rather smooth functionals of heat flux. The differences will be only in the form of the source in Eq. (14).

Conclusions. The temperature error at a certain coordinate-time point can be calculated from the error of the initial data by solving the conjugate equation. In this case, the total expenditures of the computation time correspond to two calculations of the temperature field.

NOTATION

C, heat capacity, kJ/(kg·K); H_{ij}, Hessian; L, Lagrangian; M, number of tests; N_t, number of nodes of heat-flux approximation over time; N_x, number of nodes along the coordinate; Q_{w}, heat flux, kW/m^2; S, sensitivity function; t, time; t_k, duration of the process; T, temperature, K; T^{err}, temperature in the presence of the error, K; T_0, initial temperature, K; x, coordinate, m; U, governing parameters involving the error; X, specimen thickness, m; δ, Dirac delta function; δQ, heat-flux error; ΔT, temperature increment; ε, functional of discrepancy; λ, thermal conductivity, kJ/(m·K); λ_0, parameter specifying thermal conductivity; ρ, density, kg/m^3; τ, auxiliary time; σ, standard deviation of

the error of the initial data; Ψ, conjugate temperature. Sub- and superscripts: est, estimated point; *i*, number of the time node; *j*, number of the coordinate node; *k*, *l*, current indices; w, wall; err, error.

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