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METHOD OF LINES IN DISTRIBUTED PROBLEMS OF EXPERIMENTAL DATA PROCESSING

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ABSTRACT

In many cases, the mathematical support of non-stationary thermal experiments is based on methods for solving the inverse heat conduction problem (IHCP), which include boundary thermal conditions determination, identification of heat and mass transfer processes, restoration of external and internal temperature fields, etc. However, at present, the main field of the IHCP application remains the processing and interpretation of the results of the thermal experiments. It was here where the most considerable theoretical and applied successes were achieved in methods' effectiveness and the breadth of their practical use. This paper highlights the issues of mathematical modeling of multidimensional non-stationary problems of metallurgical thermophysics.

The primary research purpose aims at solving problems associated with identifying parallel structures of algorithms and programs and their reflection in the computers' architecture in solving a wide range of applied problems. Supercomputers are currently inaccessible due to the enormous cost and service price. In this regard, a real alternative is cluster-type computing systems by which the simulation results are covered in this paper.

Being a relatively new technology, cluster-type parallel computing systems are useful in solving a large class of non-stationary multidimensional problems, while allowing to increase the productivity and quality of computations. The software developed in this paper can be used to plan and process the results of a thermophysical experiment. The algorithms developed in the application program package are simply reconstructed to solve other coefficient and boundary problems of thermal conductivity. The developed algorithms for solving thermophysical problems are highly accurate and efficient: the test solution for IHCP with accurate input data coincides with the thermophysical features of the sample material. The developed software for processing the results of a thermophysical experiment is self-regulating. Moreover, it is quite merely tuned to the solution of others and, in particular, of boundary IHCP.

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Introduction. In metallurgical production, they face many diverse and interconnected processes. It includes heat transfer and mass exchange, hydrodynamic processes in melts, as well as a change in the substance aggregation state, deformation phenomena under power and thermal loads, etc. Most of these processes can be described based on differential equations of continuum mechanics, which reflect the objective laws of conservation of mass, momentum, and energy. In mathematical

terms, these are systems of multidimensional nonlinear differential equations that, like laws of chemistry and thermodynamics, describe interconnected processes, as well as their interaction.

Moreover, the practice of recent years shows that neither the intensification of the metallurgical production processes nor the constructive improvement of metallurgical equipment variety is possible without studying and analyzing the phenomena of heat transfer by methods of mathematical modeling [1, 2]. A theoretical study of the heat and mass transfer process is mainly based on their numerical simulation using computer technology. Besides, fundamental problems in the potentially endless increase of peak computer performance disappear with the development of cluster computing systems. Parallel computing systems are developing very fast, and with the advent of computing clusters [3, 4], parallel computing has become available to many. As a rule, mass processors, standard network technologies, and freely distributed software are used to build clusters. It was these circumstances that made the so-called big problems of metallurgical thermophysics [5 – 7] possible to solve.

At the same time, the problems arising in the development of parallel computing systems that meet unique features are, as a rule, paramount and require in-depth study and research [8, 9]. Indeed, distributed computer modeling covers the whole spectrum of modern computer technology: supercomputers, cluster computing systems, local and global networks. Besides, distributed modeling allows solving problems requiring huge processing time, integrate mathematical models that are processed on various (including geographically distant) computing systems.

In many cases, the mathematical support of non-stationary thermal experiments is based on methods for solving the inverse heat conduction problem (IHCP), which include boundary thermal conditions determination, identification of heat and mass transfer processes, restoration of external and internal temperature fields, etc. However, at present, the main field of the IHCP application remains the processing and interpretation of the results of the thermal experiments.

This paper highlights the issues of mathematical modeling of multidimensional non-stationary problems of metallurgical thermophysics.

The primary research purpose aims at solving problems associated with identifying parallel structures of algorithms and programs and their reflection in the computers' architecture in solving a wide range of applied problems.

Mathematical Formulation of Research Problem. When solving IHCP, it is first of all necessary to illuminate the controllability conditions of mathematical models (MM) that allow, by methods of mathematical modeling, bringing the system into a given thermal state using control actions. We will proceed from the fact that MM is known and includes several causal features, which we denote by the *R*-input parameters' vector. Let a discrete analog of MM and a computational algorithm be developed. The MM sensitivity to vector *R* variations, i.e., it is shown that the desired solution to a specific MM problem is determined not only by the functions of spatial coordinates and time but also by the *R*-input parameters' function. Thus, to evaluate the reliability of the obtained MM solution, it is necessary to study its behavior with variations in the input data. When studying the MM sensitivity, variations in input parameters are assumed to be given. Equally important are the formulation and methods of solving inverse problems, which essence is to evaluate the vector *R* input parameters from the actual information about the simulated system known from the experiment. The mathematical modeling process of this class of problems involves several stages.

First, the development of an algorithm and a computational program for solving the direct MM problem, the computational algorithm for solving that implements the transformation.

$$T = (x, t, R) \tag{1}$$

determining the MM temperature state vector as a function of independent variables and input parameters of the vector *R*.

Secondly, when solving IHCP as a quality criterion for identifying the parameters *R* on MM solutions, it is necessary to introduce into the algorithm a particular functional characterizing the model as a whole or the deviations between the measured $T_e(t_j)$ and the computed values of the state vector $T_p(t_j)$. Let us choose the standard mean square residual as deviation the measure.

$$(T_p, T_e) = (T_p - T_e)^2, \tag{2}$$

wherein T_p is the thermal state vector value computed by the MM model. The components of the $T_e(t_j)$ vector can be determined on a discrete set of points of a given domain of temperature function definition. As a rule, in practice, several such criteria are used for the model's quality assessment.

Thus, we have come to one of the promising directions in solving IHCP corresponding to their extreme formulation using well-known numerical methods of optimization theory. Considering that the computation of the vector *gradJ()* inherent in these methods is a serious mathematical problem, we show how this can be avoided. Note that if MM implements transformation (1), then at each step of such transformations, it is possible to compute the values of functional (2). It allows, by repeated variation of the vector *R* input parameters, constructing a sequence of changes in functional (2) that would include the point of its minimum. Thus, if this is feasible, then the IHCP solution is reduced to minimizing the function of many variables. This algorithm most looks merely for one variable of the vector *R*. The solving IHCP algorithm, in this case, includes separation of the interval containing the minimum functional point and the procedure for its refining. The update of the minimum coordinate can be implemented as follows. Suppose that the functional *J(R)* (2) has a sufficient analyticity margin concerning the vector *R* input parameters. Let us represent its value by a segment of the Taylor series near a minimum.

$$J_{p+\varepsilon_{k,}1}(R) = J_{p,1} + \varepsilon_R J_{p,2} + \varepsilon_R^2 J_{p,3} + ..., \tag{3}$$

wherein

$$\begin{aligned} &\varepsilon_R = \frac{R - R_p}{R_{p+1} - R_p} \in [-1,+1], \\ &J_{p,2} = (J_{p+1,1} - J_{p-1,1})/2, \\ &J_{p,2} = (J_{p+1,1} + J_{p-1,1} - 2J_{p,1})/2 \end{aligned} \tag{4}$$

are known Taylor components, and *p=1,2,3, ...* are the numbers of grid nodes.

Having saved three terms in (3), differentiating concerning $\mathcal{E}_R$, and equating to zero, we construct the interpolation formula

$$R = R_p - \frac{(R_{p+1} - R_p)}{2} \cdot \frac{J_{p,2}}{J_{p,3}}, \tag{5}$$

wherein all the notations correspond to those adopted above. Thus, the IHCP solution from this class of problems reduces to separating the minimum and its refinement by iterations according to formula (5). This algorithm is tested below on solutions of coefficient IHCP.

Construction Features of the Controlled MM for the Coefficient IHCP Problem. Let us consider the one-dimensional problem of unsteady heat conduction described by the quasilinear equation.

$$C_{UV}(T)\frac{\partial T}{\partial \tau} = \frac{1}{x^K}\frac{\partial}{\partial x}\left[x^K\left(\lambda(T)\frac{\partial T}{\partial x}\right)\right], x \in [0,1], \tau \in [0,\infty), \tag{6}$$

wherein

$$\begin{aligned} &\tau = a_0 t / L^2, a_0 = \lambda_0 / C_{\upsilon 0}, \\ &x = x / L, C_\upsilon = C_\upsilon / C_{\upsilon 0}, \\ &\lambda = \lambda / \lambda_0, k = \overline{0,1,2}, \end{aligned} \tag{7}$$

are dimensionless input data, *k* is a parameter of the sample (plate, cylinder, and ball) shape.

Equation (6), after time discretization, is transformed at grid domain nodes (*p=1,2,…,m_x-1*) into an ordinary differential equations system of a two-point type.

$$T''_{p+\varepsilon_x,1}(\varepsilon_x) + 2A_p T'_{p+\varepsilon_x,1}(\varepsilon_x) - B_p T_{p+\varepsilon_x,1}(\varepsilon_x) = B_p TO_{p+\varepsilon_x,1}(\varepsilon_x), \tag{8}$$

wherein

$$\left.\begin{aligned} A_p &= \frac{1}{2}\left(\frac{\lambda_{p,2}}{\lambda_{p,1}} + k\frac{Dx1}{x_p}\right) \\ B_p &= \frac{Dx1}{Dt1}\frac{CV_{p,1}}{\lambda_{p,1}} \end{aligned}\right\}. \tag{9}$$

The functions $T_{p+\varepsilon_{x,}1}(\varepsilon_x), TO_{p+\varepsilon_{X},1}(\varepsilon_x)$ in (9) are assigned to the current and previous time layers, respectively.

The solution of the investigated differential equation according to the direct method is presented in an analytical form by nodes

$$T_{p+\varepsilon_x,1}(\varepsilon_x) = T^*_{p+\varepsilon_x,1}(\varepsilon_x) + C_p e^{\beta_1 \varepsilon_x} + D_p e^{-\beta_2 \varepsilon_x}, \tag{10}$$

wherein

$$\beta_1 = \Omega_p - A_p, \quad \beta_2 = \Omega_p + A_p, \quad \Omega_p = \sqrt{A_p^2 + B_p}, \tag{11}$$

are the roots of the characteristic equation;

C_p, D_p are the integration constants;

$T^*_{p+\varepsilon_{X1}}(\varepsilon_X)$ is a particular solution to the inhomogeneous equation (8).

The final sub-node solution to this problem takes the following form

$$T_{p+\varepsilon_x,1}(\varepsilon_x) = T^*{}_{p+\varepsilon_x,1}(\varepsilon_x) + F1\frac{e^{-\beta_1(1-\varepsilon_x)}}{Det}(1-e^{-2\Omega_p(1+\varepsilon_x)}) + \\ + F2\frac{e^{-\beta_1(1+\varepsilon_x)}}{Det}(1-e^{-2\Omega_p(1-\varepsilon_x)}), \tag{12}$$

wherein

$$F1 = (T_{p+1,1} - T^*_{p+1,1}), F2 = (T_{p-1,1} - T^*_{p-1,1}), Det = (1-e^{-4\Omega_p}) \tag{13}$$

are the grid complexes.

Setting in (12) $\mathcal{E}_x=0$, we obtain MM algebraic analog in the form of a system of linear differential equations of a tridiagonal structure

$$C_p T_{p+1,1} - T_{p,1} + D_p T_{p-1,1} = f_{p,1}, \quad p = \overline{1,2m-1}, \tag{14}$$

wherein

$$\left.\begin{aligned} C_p &= \frac{e^{-\beta_1}}{1+e^{-2\Omega_p}} \\ D_p &= \frac{e^{-\beta_2}}{1+e^{-2\Omega_p}} \\ f_{p,1} &= (C_p T^*_{p+1,1} - T^*_{p,1} + D_p T^*_{p-1,1}) \end{aligned}\right\}. \tag{15}$$

The quadratic dependence of the argument $TO_{p+\varepsilon_{X1}}(\varepsilon_X)$ concretizes the form of the initial function $\mathcal{E}_x$

$$TO_{p+\varepsilon_x,1}(\varepsilon_x) = TO_{p,1} + \varepsilon_x TO_{p,2} + \varepsilon^2{}_x TO_{p,3}, \tag{16}$$

wherein

$$\left.\begin{aligned} TO_{p,2} &= \frac{1}{2}(TO_{p+1,1} - TO_{p-1,1}) \\ TO_{p,3} &= \frac{1}{2}(TO_{p+1,1} + TO_{p-1,1} - 2TO_{p,1}) \end{aligned}\right\}. \tag{17}$$

Considering these dependencies, particular solution of inhomogeneous equation (8), which is included in the MM (14) in an implicit form, takes following form

$$TO^*_{p+\varepsilon_x,1}(\varepsilon_x) = M_0 + \varepsilon_x M_1 + \varepsilon^2{}_x M_2, \tag{18}$$

wherein

$$\left.\begin{aligned} M_0 &= TO_{p,1} + b_1 TO_{p,2} + 2b_2 TO_{p,3} \\ M_1 &= TO_{p,2} + b_1 TO_{p,3} \\ M_2 &= TO_{p,3} \\ b_1 &= 2\frac{A_p}{B_p}, b_2 = 4\frac{A_p^2}{B_p^2} + \frac{1}{B_p} \end{aligned}\right\}. \tag{19}$$

The solution of linear algebraic equations system (14) for given input data is entirely simply implemented by the sweep method. Thus, we can assume that we developed the first MM being necessary to solve the coefficient IHCP in the above (extreme) statement. Let us designate it as Model 1. We should also add its gradient analog to the (temperature) MM (14). By differentiating function (12) $\mathcal{E}_x$ concerning and setting $\mathcal{E}_x=0$, we construct the gradient Model 2

$$T_{P,2}(\varepsilon_x)_{\varepsilon_x=0} = \left\{T^*_{P,2}(0) + F1\frac{\ell^{-\beta_1}}{Det}\left[\beta_1 + \beta_2\ell^{-2\Omega p}\right] - F2\frac{\ell^{-\beta_2}}{Det}\left[\beta_2 + \beta_1\ell^{-2\Omega p}\right]\right\}, \tag{20}$$

wherein the function $T^*_{p+\varepsilon 2}(\varepsilon_X)$ is computed by the formula

$$T^*_{p+\varepsilon_x,2}(\varepsilon_X) = M_1 + 2\varepsilon_X M_2. \quad (21)$$

Thus, the identification MM, which includes Model 1 (14) and Model 2 (20), allows formulating a solution to the coefficient IHCP in an extreme setting according to the scheme described above.

The proposed approach is implemented as a package of application programs.

The Solution of the Test Coefficient IHCP Using Mathematical Modeling. As a test problem let us consider a cylindrical sample made of a material with thermophysical properties [16] (coke from gas coal p. 41, Table 42-molded coke):

$$\lambda = 0.161 + 0.024 \cdot 10^{-2} \cdot T$$
$$C = 1.281 + 0.208 \cdot 10^{-2} \cdot T, \quad (22)$$

The density of coke from gas coal $p = 1912, kg/m^3$. With such thermophysical properties, we simulated the temperature field of a cylindrical shape sample *(k=1)*. For given time-linear temperature change at sample boundary $(TL = 20 + 100 \cdot \tau)$, the temperature field for a particular time moment $\tau = a_0 t / R^2 = 0.5$, wherein $a_0 = \lambda_0 / p\, c_0 (\lambda_0 = 1, c_0 = 1)$, shown in Fig. 1 - 3.

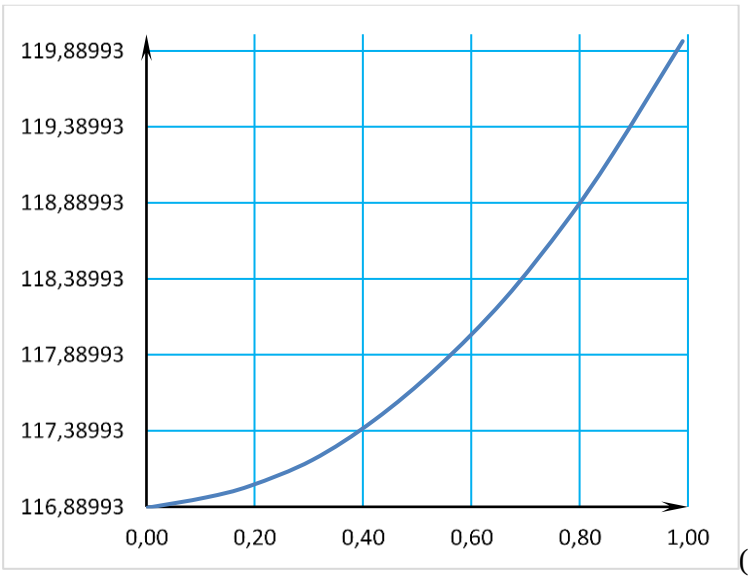

Fig. 1. The change in temperature over the at time moment $\tau = \tau_1 = 0,5$

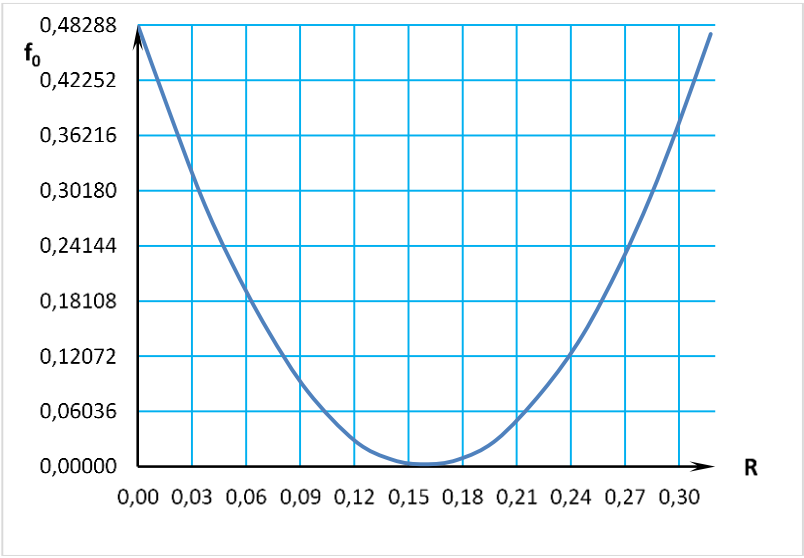

Fig. 2. The solution of the coefficient cross-section of the sample IHCP with $R = \lambda$

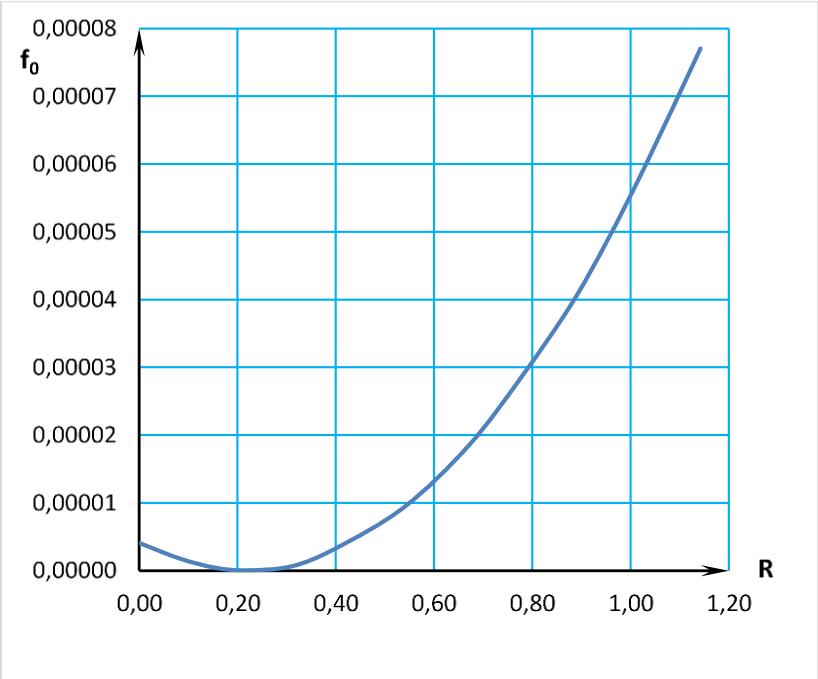

Fig. 3. The solution of the coefficient IHCP with $R = a$ *with control relative to the coefficient of thermal diffusivity*

The coefficient exact values of thermal conductivity and thermal diffusivity are respectively equal $\lambda(f_2) = 0.166, a(f_2) = 0.054$, wherein f_2 is the temperature change in the second node along the cross-section of the sample. The minimum residuals presented in Fig. 2, 3 exactly correspond to these values.

Conclusions. In many cases, the mathematical support of non-stationary thermal experiments is based on methods for solving the inverse heat conduction problem (IHCP), which include boundary thermal conditions determination, identification of heat and mass transfer processes, restoration of external and internal temperature fields, etc. However, at present, the main field of the IHCP application remains the processing and interpretation of the results of the thermal experiments. It was here where the most considerable theoretical and applied successes were achieved in methods' effectiveness and the breadth of their practical use. This paper highlights the issues of mathematical modeling of multidimensional non-stationary problems of metallurgical thermophysics.

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