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A method for reconstructing models of heat and mass transfer from the spatio-temporal distribution of parameters

© N.Y. Bykov[1,2], A.A. Hvatov[2], A.V. Kalyuzhnaya[2], A.V. Boukhanovsky[2]

[1] Peter the Great Saint-Petersburg Polytechnic University, St. Petersburg, Russia
[2] ITMO University, St. Petersburg, Russia
E-mail: nbykov2006@yandex.ru

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An algorithm of the generative design method for reconstruction of heat transfer models from the available data is proposed. The method is applied to generate a partial differential equation describing the process of heating and evaporation of a metal, the surface of which is heated by laser radiation. The high efficiency of the method was demonstrated for the purpose of reconstructing the correct structure of the equation, indicating additional processes accompanying heating as phase transitions, and also for determining the values of the temperature-dependent coefficients of the derivatives.

Keywords: Generative design method, data-driven model, laser heating, heat conduction equation.

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From the point of view of the development of artificial intelligence (AI) technologies, of particular interest is the development of methods for reconstructing models of processes of various nature in the form of partial differential equations (PDE) based on available data [1]. This approach (hereinafter referred to as the generative model design (GMD) method) seems to be extremely promising for solving a wide range of heat and mass transfer problems. The development of the GMD algorithm in relation to heat transfer problems will allow, according to available data, to clarify the structure of the PDE describing the thermal process, to identify the presence of „hidden“ accompanying processes, such as phase transformations and chemical reactions, and in some cases to describe complex phenomena with unknown properties of the objects under consideration with simpler models. From the point of view of clarifying the structure of the equations, as an example, we can cite the need to take into account the second derivative of temperature in time in „classical“ heat transfer equation for the correct description of high-intensity non-stationary processes, thermal processes in objects with strong internal heterogeneity or in small-sized objects [2]. In the case of a moving medium, the heat transfer equation is expanded by adding a convective term. Thus, in the presence of data on the thermal process (for example, the temperature distribution in the medium at different points in time), the artificial intelligence algorithm must first correctly identify the structure of the equation (the number and type of the main terms), and then determine the necessary coefficients for each structural element.

The objectives of this work are 1) development of an original recovery algorithm based on the model data in the form of the PDE in relation to solving thermal problems; 2) demonstration of the possibilities of applying the proposed approach.

The developed algorithm of the GMD method provides for the implementation of several stages of reconstruction of the unknown structure of the equation according to the available data. First, the full possible template of the desired equation is written. In this paper, we consider a general template of the thermal conductivity equation describing pulsed heating of a material by a surface heat source [3]:

$$-\frac{\partial T}{\partial t}+\frac{1}{c\rho}\frac{\partial}{\partial x}\lambda\frac{\partial T}{\partial x}+\omega\frac{\partial T}{\partial x}=0. \quad (1)$$

Here is t — time, x — coordinate. The coordinate system is associated with a moving (at a velocity of ω in the presence of evaporation) target surface. The thermal conductivity coefficient λ is considered unknown. For this coefficient, a polynomial dependence on temperature is assumed with unknown coefficients β: $\lambda=\beta_0+\beta_1T+\beta_2T^2+\beta_3T^3$. The contribution of the convective term determined by the coefficient ω is also unknown. The density ρ and the heat capacity of the material c are assumed to be constant and given. The power of the surface heat source q_s, which determines the boundary condition at $x=0$, is assumed to be known.

For the application of statistical learning methods [4] a discretized finite difference method the option of the expression (1) can be written as

$$\mathbf{Y}=\alpha_0\mathbf{E}+\sum_{p=2}^{P_t}\alpha_p\mathbf{V}_p, \quad (2)$$

where $\mathbf{Y}=-\alpha_1\mathbf{V}_1$, $\alpha_0=0$, $\alpha_1=-1$, $\alpha_p=\beta_{p-2}/(c\rho)$ for $2\leqslant p\leqslant 5$, $\alpha_6=\omega$, $\mathbf{E}$ — a vector with all components equal to one. The components of the vectors $\mathbf{V}_p$ contain the difference patterns of the elements of the equation (1) corresponding to the internal nodes of the grid and the considered moments of time. The number of components is equal to $n = (N - 2)L$ (N — the number of grid nodes of a uniform grid, L — the number of time slices for which the temperature values in the nodes are known). The number of summands P_t depends on the number of summands of the original PDE and the degree of the polynomial describing the dependence $\lambda(T)$. For the considered case of a polynomial of the third degree $P_t = 6$. Coefficients α_p ($p > 1$) are unknown and subject to definition.

Further implementation of the GMD algorithm involves two stages.

1. The components of the vectors $\mathbf{V}_p$ are calculated from the initial synthetic data (temperature distributions in grid nodes for different time slices).

2. To (2), the procedure for selecting the optimal subset of variables [4] is applied, which allows us to filter out insignificant terms and determine the necessary coefficients. In our case, the number of variables (predictors) for internal nodes is $P = P_t - 1 = 5$. The procedure involves iterating through $2P$ possible layouts (2) with one, two, three, etc., up to P terms (elements). For each fixed number of terms p, possible options of elements are sorted out and the optimal model is selected based on the calculation of the smallest sum of the square of the residuals (RSS). Next, the only optimal model is selected using the criterion BIC [4], calculated as

$$\mathrm{BIC} = n \ln(\mathrm{RSS}/n) + k \ln n, \ \ k = P + 2.$$

In this paper, statistical analysis is performed using the package R [5].

Synthetic data (spatial distributions of material temperatures for different time slices) were obtained by numerical

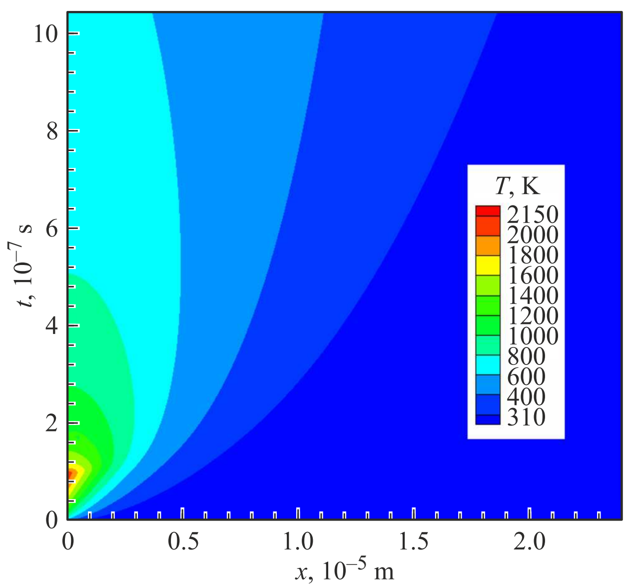

Figure 1. The spatiotemporal temperature distribution for option 2.

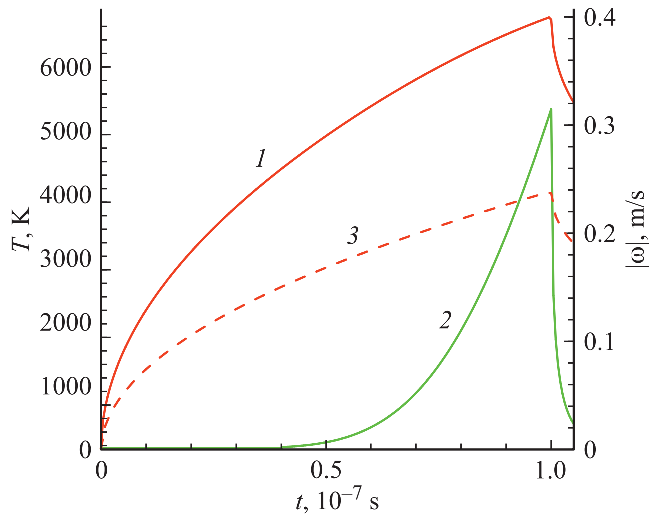

Figure 2. Change in surface temperature (*1*, *3*) and evaporation front velocity (*2*) for options 3 (*3*) and 4 (*1*, *2*).

solution (1) using the finite-difference Krank–Nicholson [2] scheme (Table 1). The boundary and initial conditions have the form [3]:

$$T(x, 0) = T_0,$$

$$-\lambda \frac{\partial T}{\partial x}\bigg|_{x=0} = q_s - L\rho\omega, \qquad T(\infty, t) = T_0, \qquad (3)$$

where L — latent heat of evaporation, $q_s = (1 - R_f)I_0$, $R_f = 0.77$ [6] — reflection coefficient, I_0 — radiation intensity on the target surface, $T_0 = 300$ K. The velocity of the surface ω corresponds to the Hertz law [3,6]. Duration of the laser pulse ($I_0 \neq 0$) — 100 ns, the radiation intensity is assumed to be constant in time, the target material is — niobium. In options 1 and 2, the material is heated below the melting point. For this case, the dependence of the thermal conductivity coefficient on the temperature is taken into account according to [7]. In options 3 and 4, the surface temperature of the material approaches or exceeds the boiling point. Taking into account the lack of reliable data for this range, the thermal conductivity of the material is considered constant and equal to the thermal conductivity of the liquid metal [7]. It should be noted that in order to simplify the formulation, the solid–liquid phase transition is not considered in the work. Examples of synthetic data are shown in Fig. 1, 2.

In this paper, data corresponding to a single temporal slice is used to generate the model (Table. 1) containing three nearby time layers (time step between layers $\Delta t = 10^{-11}$ s for options 1–4, $\Delta t = 10^{-10}$ s for option 5). The number of degrees of freedom (nodes of the spatial grid with a known temperature value) used to generate the model is 580–16,000, depending on the option (Table 1).

First, the GMD method was applied to reconstruct the equation from the data assuming that the target is heated to temperatures less than 2300 K (options 1 and 2) and the temperature dependence of the thermal conductivity

Table 1. Options of synthetic data on the target heating process

Option	Tempóral slice, μs	$I_0(t)$, W/m^2	ρ, kg/m^3	C, J/(kg $\cdot$ K)	λ, W/(m $\cdot$ K)	N_d
1	0.01	$3 \cdot 10^{11}$	8570	263	Var	998
2	1	$3 \cdot 10^{11}$	8570	263	Var	11704
3	0.0975	$7 \cdot 10^{11}$	7580	449.9	65	3224
4	0.0975	$12 \cdot 10^{11}$	7580	449.9	65	3355
5	1	$3 \cdot 10^{11}$	8570	263	Var	580

Note. N_d — number of degrees of freedom, Var — variable.

Table 2. Results of applying the optimal subset selection procedure for option 1

	α_2	α_3	α_4	α_5	α_6	BIC
Theory	*	*	*	*		
(1)	*					−3628.851
(2)	*				*	−10980.495
(3)	*	*			*	−12940.783
(4)	*	*	*	*		**−29934.639**
(5)	*	*	*	*	*	−29928.260

Table 3. Results of the GMD application

	α_0	α_1	α_2	α_3	α_4	α_5	α_6
Theory	0	−1	$2.2845 \cdot 10^{-5}$	$2.9668 \cdot 10^{-9}$	$2.9513 \cdot 10^{-12}$	$-1.0009 \cdot 10^{-15}$	0
Option 1	$2.2415 \cdot 10^{-5}$	−1	$2.2845 \cdot 10^{-5}$	$2.9669 \cdot 10^{-9}$	$2.9513 \cdot 10^{-12}$	$-1.0009 \cdot 10^{-15}$	0
Option 2	$1.2132 \cdot 10^{-7}$	−1	$2.2845 \cdot 10^{-5}$	$2.9668 \cdot 10^{-9}$	$2.9513 \cdot 10^{-12}$	$-1.0009 \cdot 10^{-15}$	0
Option 5	$-2.5967 \cdot 10^{-7}$	−1	$2.2845 \cdot 10^{-5}$	$2.9668 \cdot 10^{-9}$	$2.9513 \cdot 10^{-12}$	$-1.0009 \cdot 10^{-15}$	0
Theory	0	−1	$1.9060 \cdot 10^{-5}$	0	0	0	–
Option 3	$7.3003 \cdot 10^{-6}$	−1	$1.9060 \cdot 10^{-5}$	0	0	0	0
Option 4	$1.4656 \cdot 10^{-5}$	−1	$1.9060 \cdot 10^{-5}$	0	0	0	0.283

coefficient. In Table 2, as an example of the application of the procedure for selecting the optimal subset of elements, the results for option 1 corresponding to the irradiation stage are presented. In the first column, the number in parentheses means the number of p elements included under the sum sign on the right side of the expression (2). For this option, the procedure correctly reproduces the structure of the equation, which includes four terms (excluding the term corresponding to α_1). The minimum value of the BIC criterion corresponds to such a set of equation elements. Option 2 corresponds to the same conditions, but a longer process time $t = 10^{-6}$ s. The temperature of the material decreases due to the process of heat diffusion into the depth of the target. By time 1 μs, the temperature range of the material is 300−800 K, while the number of degrees of freedom increases to 12 000. The convective term for this option is also not reproduced.

The results of using the GMD method for options 1 and 2 are summarized in Table 3. In the first row of the table (graph „Theory"), the normalized coefficients $\alpha_2 - \alpha_5$ are given, corresponding to the approximation of the thermal conductivity coefficient used in the numerical solution of equation (1). The following lines contain the reconstructed coefficients for the considered options. As follows from the presented results, the values of the coefficients in the polynomial dependence of thermal conductivity are reproduced fairly accurately. The error of restoring the total coefficient of thermal conductivity does not exceed 0.002%. Increasing the time step to 10^{-10} s and grid pitch 50 times up to 10^{-7} m did not affect the model recovery results (option 5, Table 3).

To demonstrate the capabilities of the GMD to indicate the flow of additional physical processes, the model was restored for options 3 and 4. In option 3, the intensity of laser radiation was insufficient for evaporation of the target surface. The surface temperature reaches 4000 K (Fig. 2). For option 4, the surface temperature by the time the pulse is completed exceeds 6000 K and the evaporation front velocity becomes significant (Fig. 2).

The results of using GMD for options 3 and 4 are shown in Table 3. It can be seen that the GMD correctly restores the structure of the equation. For option 4, the coefficient for the convective term is reproduced. The value of the dimensionless thermal conductivity coefficient is also reproduced correctly.

The conducted research is the first stage in the study of the possibilities of using the proposed GMD algorithm both for the direct construction of a mathematical model of a complex phenomenon according to available data, and for the indication of related processes, such as, for example, phase transformations, as well as to clarify the thermophysical parameters of materials. The next important step in the study of the effectiveness of the generative design algorithm for reconstructing models of thermal processes will be its approbation on noisy experimental data.

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Conflict of interest

The authors declare that they have no conflict of interest.

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