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SEQUENTIAL MODELS OF PHYSICAL PHENOMENON AND THE JUSTIFICATION OF MATHEMATICAL MODELING

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Abstract. The substantiation of passing to the limit to the balance relations in the determination of the mathematical models is proposed. This is based on the sequential method.

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1. Introduction

The standard method of the determination of mathematical models begins with the selection of the given area in the elementary volume. Then the balance relations are obtained there with using of physical laws. The next step is passing to the limit as this volume is compressed to a point. The equations that are the result of this transformation are the base of the mathematical model.

It should be noted that there is a step, requiring the strictly justification. This is the passage to the limit, one of the most important mathematical procedures, to which decided to treat with the utmost care. The assumption of the high smoothness of the considered state function is usually used here (see, for example, [8]).

The smoothness of the state of the system corresponds to the notion of the classic solution of mathematical physics problems. It can be proved by means of the theory of the considering equations (see, for example, [2]). However, this is done after the equation was obtained. This theory does not apply at the stage of construction of the mathematical model.

We could consider also the generalized solution of mathematical physics problems. This is based on the theory of distributions (see, for example, [9]). The generalized solution uses weaker requirements for the parameters of the problem than the classic one (see, for example, [2]). The integral relations that determine the generalized solution have the directly physical sense. However, it uses a priori assumption about the properties of the state function too.

We propose a method of mathematical modeling that requires no a priori assumptions about the properties of the state function of the system. This is based on the sequential technique. This is an analogue of the proof of the completion theorem (see, for example, [3]) and the alternative theory of distributions [1]. The practical implementation of this approach is an analogue of the convergence justification for the finite difference method (see, for example, [4]). The idea of the sequential justification of mathematical modeling is used in [7]. We illustrate it in the simplest example of the heat transfer process.

2. Simplest classic mathematical model of the heat transfer phenomenon

Consider the stationary heat transfer phenomenon for the one-dimensional case. Suppose there exists a source of heat. Then the change of the quantity of heat on an interval $\left[x, x+h\right]$ is

$$q(x) - q(x+h) = \int_x^{x+h} f(\xi)\, d\xi, \tag{1}$$

where the known function f characterizes the density of the source of heat. The flux of heat at the concrete point x is proportional to the difference between the temperature u at this point and at the previous point $x–h$. If the length h is small enough, then the value q can be determined by Fourier law

$$q(x) = -k(x)\frac{u(x) - u(x-h)}{h}, \tag{2}$$

where k is the coefficient of the heat conductivity.

Suppose the function u is twice continuously differentiable. From the equalities (1), (2) after passing to the limit as $h \to 0$ it follows the equality

$$\frac{d}{dx}\left[k(x)\frac{du(x)}{dx}\right] = f(x),\ x \in (0, L), \tag{3}$$

where L is the length of the body. This is the stationary one-dimensional heat equation. Let the temperature at the ends of the body is zero. Then we obtain the boundary conditions

$$u(0) = 0,\ \ u(L) = 0. \tag{4}$$

The boundary problem (3), (4) is the mathematical model of the considered phenomenon under the given suppositions.

The twice continuously differentiable function on the interval $[0,L]$ that satisfies the equalities (3), (4) is called the *classic solution* of this problem. We can prove that the problem (3), (4) has a unique classic solution under some suppositions about the known functions k and f (see, for example, [8]).

Use the finite difference method for finding the approximate solution of this problem. Divide the interval $(0,L)$ into M equal parts. Determine the step $h = L/M$ and the points $x_i = ih,\ i = 0, ..., M$. Determine the standard difference operators

$$\delta_{\bar{x}} : \mathbf{R}^{M+1} \to \mathbf{R}^M,\ \ \delta_x : \mathbf{R}^{M+1} \to \mathbf{R}^M$$

by the equalities

$$\delta_{\bar{x}} v_i = \left(v_i - v_{i-1}\right)/h,\ i = 1, ..., M;\ \delta_x v_i = \left(v_{i+1} - v_i\right)/h,\ i = 0,\ ..., M-1,$$

where $v_i = v(x_i)$. If the function $v = v(x)$ is continuously differentiable, then these formulas approximate its derivative at the point x_i.

The classic solution of the problem (3), (4) is continuously twice differentiable. We approximate the equation (3) by the equality

$$\delta_x\left(k_i\delta_{\bar{x}}u_i\right) = f_i,\ i = 1,...,M-1, \tag{5}$$

where

$$u_i = u(x_i),\ k_i = k(x_i),\ f_i = \frac{1}{h}\int_{x_i}^{x_{i+1}} f(\xi)\,d\xi.$$

We add also the boundary conditions

$$u_0 = 0,\ u_M = 0. \tag{6}$$

The system of linear algebraic equations (5), (6) can be solved by means of the marching method. Therefore, we find all values u_i, namely the grid function. Then we determine its linear interpolation

$$u_h(x) = u_i + x\delta_x u_i,\ x \in (x_i, x_{i+1}),\ i = 1,...,M-1. \tag{7}$$

For the justification of the finite difference method, it is necessary to prove the convergence $u_h \to u$ in the class of the twice continuously differentiable functions as $h \to 0$, where the limit u is the classic solution of our boundary problem (see [4]).

Note that we use the properties of the classic solution for the first step of analysis (this is mathematical modeling) and for the final step too. We could prove the continuously twice differentiability of the solution of the boundary problem by means of the differential equations theory. However, we can obtain this result, if the equation (3) has already given. We cannot any possibilities to use it for passing to the limit before the determination of the equation. Therefore, the problem of the justification of modeling is open.

3. Generalized model of the stationary heat transfer phenomenon

We considered the classic solution of the boundary problem. However, maybe its generalized solution will be applicable for this case. The *generalized solution* of the problem (3), (4) is an element u of Sobolev space H_0^1 of all square Lebesgue integrable functions on the interval $(0, L)$ with its first derivatives and zero values on the boundary. Besides, it satisfies the integral equality

$$-\int_0^L k(x)\frac{d\lambda(x)}{dx}\frac{du(x)}{dx}dx = \int_0^L \lambda(x) f(x)dx \quad \forall \lambda \in H_0^1. \tag{8}$$

Each classic solution of the boundary problem is its generalized solution, and the smooth enough generalized solution is the classic solution of this problem. The existence of the generalized solution is proved easier than its classic analogue. The analysis of the classic solution adds up frequently to obtaining the generalized solution and proving its smoothness. Therefore, we could suppose that generalized solution maybe applicable for the justification of mathematical modeling.

However, we have a serious objection. We consider the equality (8) as the corollary of the boundary problem (3), (4). We determine the generalized solution with respect to the equation (3) with the boundary conditions (4). We could apply the generalized solution for the justification of mathematical modeling, if it has the direct physical sense only. Try to determine the equality (8) as the corollary of the balance relations (1), (2) without using the differential equation (3).

Multiply the equality (1) by a smooth enough function λ with zero values on the boundary, and integrate the result. Dividing it by the small interval length h, we get

$$\int_0^L \frac{\lambda(x)-\lambda(x-h)}{h} q(x)\,dx + \frac{1}{h}\int_0^h \lambda(x-h)q(x)dx - \\ -\frac{1}{h}\int_L^{L+h} \lambda(x-h)q(x)dx = \int_0^L \lambda(x)\frac{1}{h}\int_x^{x+h} f(\xi)\,d\xi\,dx \ \forall\lambda. \tag{9}$$

Pass to the limit here with using of the mean theorem and the equality (2). We obtain the integral equality (8). This result is true, if the functions u and λ belong to Sobolev space H_0^1.

Thus, the equality (8) can be obtained as the corollary of the balance relations (1), (2). Therefore, it has the direct physical sense. We can interpret it as the special form of the mathematical model of the considered physical phenomenon. Now we have the following definition.

Definition 1. The boundary problem (3), (4) is called the **classic model** of the considered phenomenon, and the integral equality (8) is called its **generalized model**.

The self-determination of the generalized model is confirmed also by the possibility of its direct numerical analysis. Indeed, the standard formulas of the approximate differentiation follow directly from the definition of the generalized derivative.

Divide the given interval $(0,L)$ by M equal parts with the step h. Approximate the integrals of the equality (8) by the right rectangles formula, and approximate the derivatives there by the forward difference formula. We obtain

$$\sum_{i=0}^{M-1} k_i \frac{\lambda_{i+1}-\lambda_i}{h}\frac{u_{i+1}-u_i}{h}\ h \ = \sum_{i=0}^{M-1} \lambda_i f_i h,$$

where $\lambda_i = \lambda(x_i)$. Using the discrete analogue of the formula of integration by parts and the boundary conditions, we obtain the difference equations (5). Thus, the equalities (5), (6) are the approximation of the generalized model too. Note that the justification of the convergence of the numerical method to the generalized solution is easier than to the classic solution.

Thus, the generalized model is more preferable than the classic one. However, obtaining of the integral equality (8) as the corollary of the balance relations (1), (2) is right, if the function u belongs to Sobolev space. This set is larger than the space of the twice differentiable functions. However, we do not have any information about the properties of the state function before obtaining the mathematical model. Therefore, the generalized method is not applicable too for the justification of mathematical modeling.

4. Sequential model of the stationary heat transfer phenomenon

We have the difficulty of passing to the limit. It can be substantiated with using properties that can be obtained after passing to the limit only. We have an analogue here with the notion of the limit. This is non-constructive. If we would like to determine the convergence of the sequence to a limit, it is necessary to know this limit. However, we know as a rule the sequence only. We do not know even if this sequence is convergent or not. Therefore, the criterions of the convergence are used for the practical situation. For example, the numerical sequence is convergent, if it is fundamental, by Cauchy criterion. The notion of the fundamental sequence is constructive, because it uses the elements of the sequence only.

Unfortunately, Cauchy criterion is true for the complete spaces only. Unfortunately, the majority of the spaces are non-complete. However, the fundamental sequence is convergent always on the completion of the non-complete space. The construction of the completion uses the idea of the definition of the real numbers set by Cantor. Each element of this completion is the equivalence class of the fundamental sequences. This is the basis of the sequential method.

Try to apply the sequential method for the justification of mathematical modeling. We have an additional reason for it. The generalized solution of mathematical physics problems is based on the distributions theory. Particularly, it uses the generalized derivatives that are determined by the distributions theory technique. It is known that the distribution is a linear continuous functional on the set of the infinite differentiable compact functions [2]. However, there exists a definition of the distribution by sequential method [9]. This is an equivalence class of the fundamental sequences of the smooth enough functions. Now we use the analogical technique for the determination of the special form of the mathematical model.

Consider again the stationary heat transfer phenomenon. Divide the given interval by M equal parts with the step $h = L/M$. Determine the points $x_i = ih$, $i = 0,...,M$. Consider an elementary cell $\Omega_i = [x_{i-1}, x_i]$, $i = 1,...,M$. Denote be Γ the set of cells $\{\Omega_i\}$. The grid function on the set Γ is a vector of M+1 degree with indexes $i = 0,...,M$.

The state system in the cell Ω_i is characterized by the balance relations (1), (2), i.e.

$$q(x_i) - q(x_i + h) = \int_{x_i}^{x_i+h} f(\xi)\, d\xi, \;\; q(x_i) = -k(x_i)\frac{u(x_i) - u(x_i - h)}{h}.$$

Using the standard denotations of the difference operators, we obtain again the difference relations (5) with boundary conditions (6). Now the system (5), (6) is obtained from the physical law directly without using the boundary problem (3), (4). We do not use any mathematical suppositions here.

Find all values $u_i = u(x_i)$ from the problem (5), (6). Then determine its linear interpolation u_h by the formula (7). Now consider the sequence of positive numbers $\{h_k\}$ that tends to the zero, and the sequence of linear interpolations $\{u_{h_k}\}$.

Definition 2. If the sequence $\{u_{h_k}\}$ is fundamental with respect to a space H, then this is called the **sequential model** or more exact ***H*-sequential model** of the considered system; its equivalence class is called the **sequential state**.

Our analysis will be finish, if we determine the space H such that the sequence $\{u_{h_k}\}$ is H-sequential model of the system.

5. Justification of the sequential method

Prove the following result.

Theorem. Suppose the function k is lower bounded by a positive constant, and f is local integrable on the interval $(0, L)$ and belongs to the space H^{-1} that is adjoint to H_0^1. Then the sequence $\{u_{h_k}\}$ is the sequential model of the considered system with respect to the weak topology of the space H_0^1, and its equivalence class is the sequential state of the system.

Proof. Consider a smooth enough function λ on the interval $(0, L)$ with zero value on its boundary. Multiply the i-th equality (5) by the value $\lambda_i = \lambda(x_i)$. After summing we get the equality

$$\sum_{i=1}^{M-1} \left[\delta_x \left(k_i \delta_{\bar{x}} u_i \right) \lambda_i \right] = \sum_{i=1}^{M-1} f_i \lambda_i.$$

Using the formula of summing by parts, for all grid function $\{g_i\}$ with zero final component we have

$$\sum_{i=1}^{M-1} (\delta_x g_i) \lambda_i = \frac{1}{h} \sum_{i=1}^{M-1} (g_{i+1} - g_i) \lambda_i = \frac{1}{h} \sum_{i=1}^{M-1} g_i \left(\lambda_i - \lambda_{i-1} \right) = -\sum_{i=1}^{M} g_i \left(\delta_{\bar{x}} \lambda_i \right).$$

Then we transform the previous equality

$$-\sum_{i=1}^{M} \left(k_i \delta_{\bar{x}} u_i \delta_{\bar{x}} \lambda_i \right) = \sum_{i=1}^{M} f_i \lambda_i. \tag{10}$$

Find the derivatives

$$\frac{du_h(x)}{dx} = \delta_{\bar{x}} u_i, \quad \frac{d\lambda_h(x)}{dx} = \delta_{\bar{x}} \lambda_i, \quad x \in \Omega_i, \ i = 1, ..., M,$$

where λ_h is the linear interpolation of the grid function $\{\lambda_i\}$. Now we determine the integral

$$\int_0^L k^h \frac{du_h}{dx} \frac{d\lambda_h}{dx} dx = \sum_{i=1}^{M} \int_{\Omega_i} k^h \frac{du_h}{dx} \frac{d\lambda_h}{dx} dx = h \sum_{i=1}^{M} \left(k_i \delta_{\bar{x}} u_i \delta_{\bar{x}} \lambda_i \right),$$

where the function k^h is equal to k_i on the set Ω_i. This is the piecewise constant interpolation of the grid function $\{k_i\}$.

Determine the grid function $\{g_i\}$ from the equalities

$$g_0 = 0, \ \delta_{\bar{x}} g_i = f_i, \ i = 1, ..., M-1.$$

Using the formula of summing by parts, we get

$$\int_0^L g^h \frac{d\lambda_h}{dx}dx = \sum_{i=1}^{M}\int_{\Omega_i} g^h \frac{d\lambda_h}{dx}dx = h\sum_{i=1}^{M}\left(g_i\delta_{\bar{x}}\lambda_i\right) = -h\sum_{i=1}^{M}\left(\delta_x g_i\lambda_i\right) = -h\sum_{i=1}^{M} f_i\lambda_i,$$

where g^h is the piecewise constant interpolation of the grid function $\{g_i\}$.

Now we transform the equality (10).

$$\int_0^L k^h \frac{du_h}{dx}\frac{d\lambda_h}{dx}dx = \int_0^L g^h \frac{d\lambda_h}{dx}dx. \tag{11}$$

Choose the function λ such that its grid function $\{\lambda_i\}$ is equal to $\{u_i\}$. Then we have

$$\int_0^L k^h \left(\frac{du_h}{dx}\right)^2 dx = \int_0^L \frac{du_h}{dx}\, g^h dx. \tag{12}$$

Under supposition of the theorem, there exists a positive constant k_0 such that $k(x)\geq k_0$ for all $x\in(0,L)$. Hence, we obtain

$$\int_0^L k^h \left(\frac{du_h}{dx}\right)^2 dx \geq k_0\int_0^L \left(\frac{du_h}{dx}\right)^2 dx = k_0\left\|u_h\right\|^2_{H_0^1}.$$

Estimate the integral at the right-hand side of the equality (12).

$$\left|\int_0^L \frac{du_h}{dx}\, g^h dx\right| \leq \left\|\frac{du_h}{dx}\right\|_{L_2}\left\|g^h\right\|_{L_2} = \left\|u_h\right\|_{H_0^1}\left\|g^h\right\|_{L_2}.$$

From (12) for $h=h_k$ it follows that

$$\left\|u_{h_k}\right\|_{H_0^1} \leq \frac{1}{k_0}\left\|g^{h_k}\right\|_{L_2}.$$

Note that the derivative of the function g^h is equal to f_i on the set Ω_i. By mean value theorem, we have the convergence of the derivative of g^h to f a.e. on $(0,L)$ as $h\to 0$. Denote by f^h the generalized derivative of g^h. Using the condition $f\in H^{-1}$, we have the convergence $f^{h_k}\to f$ in H^{-1} and $g^{h_k}\to g$ in L_2 as $k\to\infty$, where the generalized derivative of g is equal to f. Then the sequence $\left\{g^{h_k}\right\}$ is bounded in L_2. From the previous inequality it follows the boundedness of the sequence $\{u_{h_k}\}$ in H_0^1. Using Banach – Alaoglu theorem, extract a subsequence that is weakly convergent in the space H_0^1. Therefore, it is fundamental with respect to the weak topology of the considered Sobolev space. By Definition 2, this is the sequential model of the system, and the relevant equivalence class is the sequential state of the system. We can obtain this result for all subsequences of $\{u_{h_k}\}$. Then the whole sequence has the same properties. This completes the proof of the theorem.

We determine the sequential model under the suppositions with respect to the given functions only. We do not have a priori assumption with respect to the state function. Therefore, our model is substantiated.

Try to determine the relations between the different forms of the mathematical models. We can apply the known results of the convergence of the finite difference method here. If the function k is continuous, then after passing to the limit at the equality (11) we obtain the equality (8) (see [4]). Therefore, we get the convergence $u^{h_k} \to u$ weakly in H_0^1, where u is the generalized state of the system. Thus, we can obtain also the standard forms of the mathematical models.

We have the following results. Under the suppositions of the theorem, we obtain the sequential model of the system and its sequential state. Under the additional assumption, we have the generalized state. This is the classical state under stronger properties of the parameters of the system. Thus, we have the equality of the three forms of the state system for the small enough parameters. Under weaker suppositions, it is possible non-existence of the classical state. However, there exist the equal generalized and sequential solutions. Using the weaker suppositions, we can have the sequential state only. Note that the standard numerical method is applicable for finding each state of the system. However, the proof of its convergence is easier for the weaker form of the model.

The sequential method was used in [6] for the extension of the optimization control problems and in [5] for the prolongation of the binary relations.

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