

THERMODYNAMIC MODELLING OF HEAT CONDUCTION

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Abstract. The paper describes a thermodynamic method for solving heat conduction problems. On the one hand, the algorithm used is based on the cellular automata technique and on the other hand, on the thermodynamic laws. The hypothesis of the local state allows us to represent every element of a continuum as a homogeneous thermodynamic system which can be considered as a cell. The state space of such cells is continuous whereas usually it is assumed to be discrete. The main advantage of this method is the absence of any partial differential equations. Therefore, the method is rather a tool for the direct simulation of a process than for the solution of partial differential equations. Two-dimensional heat conduction in solids is discussed as an example.

Key words: heat conduction, thermodynamics, cellular automata.

1. INTRODUCTION

Heat conduction is a well-known phenomenon. It is the process of energy transmission by a medium which does not involve movement of the medium itself.

Commonly, heat conduction problems are solved using the Fourier's law to a heat flux calculation [1]

$$\vec{q} = -\lambda \nabla T. \quad (1)$$

Here, λ is heat conductivity, \vec{q} is heat flux, and T is temperature.

This law holds for many media in the sufficiently small temperature gradient range. The Fourier's law leads to a parabolic field equation for the temperature

$$\frac{\partial T}{\partial t} = \frac{\lambda}{\rho c} \nabla^2 T, \quad (2)$$

where t is time, ρ is density, and c is heat capacity per unit mass.

From the physical point of view, the heat conduction equation (2) is questionable because it allows an infinite propagation speed of thermal disturbances. Attempts to eliminate the paradox are not finished yet [2-4]. The simplest generalization of the Fourier's law including relaxational effects is the Maxwell-Cattaneo equation

$$\tau \frac{\partial \vec{q}}{\partial t} + \vec{q} = -\lambda \nabla T, \quad (3)$$

with τ the relaxation time of \vec{q} . In this case, the evolution equation for the temperature is hyperbolic

$$\tau \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \frac{\lambda}{\rho c} \nabla^2 T. \quad (4)$$

However, in most problems of heat conduction, τ is found to be of the order $10^{-13} s$ to $10^{-10} s$, so it is then legitimate to use the classical Fourier rather than the Maxwell-Cattaneo equation [5].

It must be noted that the Fourier's law as well as all its generalizations connect a mechanical quantity \vec{q} with the thermodynamic temperature. Thermodynamic concepts are introduced usually into mechanical problems by means of the hypothesis of local equilibrium [6] or, as called by Kestin [7], the "principle of local state". Such a hypothesis is needed to assign to a non-equilibrium state the entropy and thermodynamic temperature of the accompanying equilibrium state.

Thermodynamic parameters of the element are considered identical to their physical parameters, such as mass and volume. However, some properties of the thermodynamic parameters expose themselves only in the Gibbsian state space. In particular, each thermodynamic parameter should have the property to be a function of state. Such a feature is often lost by pure mechanical description. Namely, as shown by Chen and Eu [8], entropy cannot become a function of state in the space of macroscopic field variables.

The interaction between elements of the continuum leads finally to the conclusion that parameters of neighbouring elements are connected by certain relations. At the same time, if they really interact, it should have the influence on their thermodynamic states. Consequently, accompanying equilibrium states of neighbouring interacting elements must also be coupled. Thus, it is of interest to determine the relations between thermodynamic parameters of interacting systems and compare them with mechanical ones.

However, as noted by Truesdell and Bharatha [9], "the formal structure of classical thermodynamics describes the effects of changes undergone by some single body. While it allows these effects for one body to be compared with corresponding effects for another body, it does not represent the effects associated with two bodies simultaneously or in any

way conjointly." Just therefore the "marriage between thermodynamics and continuum mechanics is neither simple nor straightforward" [7].

To elaborate a thermodynamic model of heat conduction, the problem of thermodynamic descriptivity is discussed in the second part of the paper. The problem is to determine the consistency between thermodynamic descriptions for the same medium by means of different partitions. Further, conditions of thermodynamic descriptivity are applied to the interaction between three neighbouring thermodynamic systems. As a result, the relation is obtained, which couples the non-equilibrium state of a system with the states of its neighbours. An algorithm of calculation of the heat conduction is elaborated on the basis of such a method of description. It is presented in the third part, where a simple two-dimensional heat conduction problem is described as an example. The proposed algorithm of calculations is similar to cellular automata rather than to methods of finite differences or finite elements. At the same time, it is not the proper cellular automaton because the states of cells are identified with thermodynamic states of elements and the rule of updating the states of the cells applied is not artificial but follows from the thermodynamic laws. The results of calculations of temperature distributions in a rectangular domain and some conclusions are presented in the fourth part.

2. THERMODYNAMIC BACKGROUND

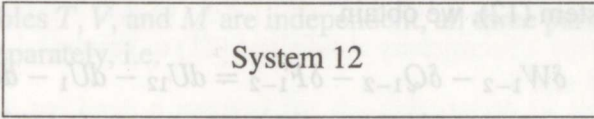
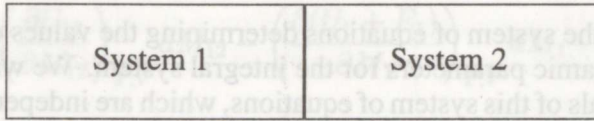
As was noted above, a problem exists in the simultaneous thermodynamic description of two or more interacting systems. The term "interacting" is very important. In fact, if two systems are fully independent, we can prescribe their states as arbitrary.

We suppose that every thermodynamic system can be considered as homogeneous, and its state is fully determined when the values of two intensive parameters are prescribed.

To obtain the simultaneous thermodynamic description of two or more interacting systems, we start with the simplest possible situation. Let us consider two interacting homogeneous thermodynamic systems 1 and 2, each of which is characterized by the same equations of state. Let the values of temperatures T_1, T_2 , and pressures p_1, p_2 , be prescribed.

If two thermodynamic systems interact with each other, it is expressed in certain interconnections between their parameters. Therefore, every variation in the values of parameters in one system leads to a certain change in the values of parameters in the other. Consequently, we can consider the integrity of such systems as a whole system. Thus, in our consideration, we include system 12, containing both system 1 and system 2.

The problem to solve is to determine the values of parameters for the integral system remaining on the thermodynamic level of description.



Since system 12 contains both system 1 and system 2, the additivity conditions should be valid for mass and volume

$$M_{12} = M_1 + M_2, \quad V_{12} = V_1 + V_2. \quad (5)$$

These definitions allow us to calculate one thermal intensive parameter of the integral system, namely, specific volume v

$$v_{12} = \frac{V_1 + V_2}{M_1 + M_2}, \quad (6)$$

as the function of state.

To determine the intensive state of the integral system completely, we need to know the value of at least one more thermal intensive parameter, namely, temperature or pressure. We define them by prescribing heat and work for the integral system

$$T_{12}dS_{12} = T_1dS_1 + T_2dS_2 - \delta Q_{1-2}, \quad (7)$$

$$p_{12}dV_{12} = p_1dV_1 + p_2dV_2 - \delta W_{1-2}, \quad (8)$$

where S is entropy, and δQ_{1-2} and δW_{1-2} are heat and work of interaction, respectively. To include the energy transport by matter, we should define in addition

$$\mu_{12}dM_{12} = \mu_1dM_1 + \mu_2dM_2 - \delta F_{1-2}, \quad (9)$$

where $\mu = pv + u - Ts$ is chemical potential, and δF_{1-2} is the material energy transfer due to interaction. In the case of equilibrium, all interaction-related quantities are equal to zero.

The latter definitions do not give us the direct method for the calculation of temperature and pressure as functions of state even if heat and work of interaction are known. Together with the fundamental Gibbs equation for each system [6]

$$T_1dS_1 = dU_1 + p_1dV_1 - \mu_1dM_1, \quad (10)$$

$$T_2dS_2 = dU_2 + p_2dV_2 - \mu_2dM_2, \quad (11)$$

$$T_{12}dS_{12} = dU_{12} + p_{12}dV_{12} - \mu_{12}dM_{12}, \quad (12)$$

they form the system of equations determining the values of the remaining thermodynamic parameters for the integral system. We will try to find the first integrals of this system of equations, which are independent of the kind of a process.

If we subtract the sum of these fundamental Gibbs equations for subsystems (10) and (11) from the fundamental Gibbs equation for the integral system (12), we obtain

$$\delta W_{1-2} - \delta Q_{1-2} - \delta F_{1-2} = dU_{12} - dU_1 - dU_2. \quad (13)$$

According to the first law of thermodynamics, the left hand side of the obtained relation is the definition of the energy of interaction between subsystems 1 and 2

$$\delta W_{1-2} - \delta Q_{1-2} - \delta G_{1-2} = -dE_{1-2}. \quad (14)$$

Therefore, the energy variation can be represented in the form

$$dU_{12} = dU_1 + dU_2 - dE_{1-2}. \quad (15)$$

Generally speaking, we could define the energy of the integral system in such a form *a priori*, however, we prefer the thermodynamic way because it allows us to consider the interaction energy as a function of state.

Due to the additivity of energy, we can expand the interaction energy into two parts, corresponding to each subsystem

$$dE_{1-2} = dE_1 + dE_2 \quad (16)$$

and rewrite the expression for energy variation in the form

$$dU_{12} = dU_1 + dU_2 - dE_1 - dE_2. \quad (17)$$

The obtained condition of energy conservation is too general for direct applications even if the energies of interaction are prescribed. To have more convenient conditions, we use the property of energy to be a function of state that allows us to represent its total differential in the form

$$dU = \left(\frac{\partial U}{\partial T} \right)_{V,M} dT + \left(\frac{\partial U}{\partial V} \right)_{T,M} dV + \left(\frac{\partial U}{\partial M} \right)_{T,V} dM, \quad (18)$$

where variables T, V, M are considered as independent. Applying this procedure to each system, we have

$$\begin{aligned} & \left(\frac{\partial U_{12}}{\partial T_{12}} \right)_{V,M} dT_{12} - \left(\frac{\partial(U_1 + E_1)}{\partial T_1} \right)_{V,M} dT_1 - \left(\frac{\partial(U_2 + E_2)}{\partial T_2} \right)_{V,M} dT_2 + \\ & + \left(\frac{\partial U_{12}}{\partial V_{12}} \right)_{T,M} dV_{12} - \left(\frac{\partial(U_1 + E_1)}{\partial V_1} \right)_{T,M} dV_1 - \left(\frac{\partial(U_2 + E_2)}{\partial V_2} \right)_{T,M} dV_2 + \end{aligned}$$

$$\begin{aligned}
& + \left(\frac{\partial U_{12}}{\partial M_{12}} \right)_{T,V} dM_{12} - \left(\frac{\partial(U_1 + E_1)}{\partial M_1} \right)_{T,V} dM_1 - \\
& - \left(\frac{\partial(U_2 + E_2)}{\partial M_2} \right)_{T,V} dM_2 = 0. \tag{19}
\end{aligned}$$

Since variables T , V , and M are independent, all three parts of (19) are equal to zero separately, i.e.

$$\begin{aligned}
& \left(\frac{\partial U_{12}}{\partial T_{12}} \right)_{V,M} dT_{12} - \left(\frac{\partial(U_1 + E_1)}{\partial T_1} \right)_{V,M} dT_1 - \\
& - \left(\frac{\partial(U_2 + E_2)}{\partial T_2} \right)_{V,M} dT_2 = 0, \tag{20}
\end{aligned}$$

$$\left(\frac{\partial U_{12}}{\partial V_{12}} \right)_{T,M} = \left(\frac{\partial(U_1 + E_1)}{\partial V_1} \right)_{T,M} = \left(\frac{\partial(U_2 + E_2)}{\partial V_2} \right)_{T,M}, \tag{21}$$

$$\left(\frac{\partial U_{12}}{\partial M_{12}} \right)_{T,V} = \left(\frac{\partial(U_1 + E_1)}{\partial M_1} \right)_{T,V} = \left(\frac{\partial(U_2 + E_2)}{\partial M_2} \right)_{T,V}. \tag{22}$$

The first of the obtained conditions depends on temperature variations and determines the heat capacity of the integral system. The third is used for entropy calculations. The second condition is most useful. In fact, due to the differential equations of thermodynamics,

$$\left(\frac{\partial U}{\partial V} \right)_{T,M} = T \left(\frac{\partial S}{\partial V} \right)_{T,M} - p = T \left(\frac{\partial p}{\partial T} \right)_v - p. \tag{23}$$

If the equations of state for the medium under consideration are known, we can calculate the value of the second intensive parameter of the integral system. Therefore, the state of the integral system is completely determined if the energy of interaction is prescribed. All together, these conditions ensure the equivalency between the thermodynamic description on the level of subsystems and that on the level of the integral system. To emphasize this fact in what follows, we call them the thermodynamic descriptivity conditions.

It must be noted that thermodynamic descriptivity conditions (20)–(22) do not only connect parameters of systems 1 and 2 with those of the integral system 12, but also parameters of systems 1 and 2 themselves. Consequently, they impose additional conditions on the thermodynamic states of interacting systems.

As an example of application, let us consider the interaction between three systems contacting each other as shown in the following figure:

System 1	System 2	System 3
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Since we deal only with thermodynamic parameters, we describe the interaction in terms of the Gibbsian state (phase) space.

In the non-equilibrium case, we should apply the general thermodynamic descriptivity conditions (21) to systems 1 and 2 as well as to systems 2 and 3

$$\left(\frac{\partial u_1}{\partial v_1}\right)_T + \left(\frac{\partial e_{12}}{\partial v_1}\right)_T = \left(\frac{\partial u_2}{\partial v_2}\right)_T + \left(\frac{\partial e_{21}}{\partial v_2}\right)_T, \quad (24)$$

$$\left(\frac{\partial u_3}{\partial v_3}\right)_T + \left(\frac{\partial e_{32}}{\partial v_3}\right)_T = \left(\frac{\partial u_2}{\partial v_2}\right)_T + \left(\frac{\partial e_{23}}{\partial v_2}\right)_T, \quad (25)$$

where e_{ij} is the interaction energy per unit mass for the system i with respect to the system j .

It must be noted that even if the explicit expressions for the interaction energies are unknown, we can determine the state of the system 2 in the case of heat conduction. To show this, we represent the thermodynamic descriptivity conditions in the form

$$\left(\frac{\partial u_1}{\partial v_1}\right)_T = \left(\frac{\partial u_2}{\partial v_2}\right)_T + \left(\frac{\partial e_{21}}{\partial v_2}\right)_T - \left(\frac{\partial e_{12}}{\partial v_1}\right)_T, \quad (26)$$

$$\left(\frac{\partial u_3}{\partial v_3}\right)_T = \left(\frac{\partial u_2}{\partial v_2}\right)_T + \left(\frac{\partial e_{23}}{\partial v_2}\right)_T - \left(\frac{\partial e_{32}}{\partial v_3}\right)_T. \quad (27)$$

Due to the symmetry of the problem of heat conduction, we have no preferences between systems 1 and 3 with respect to system 2. Consequently, their actions relative to system 2 should be equal

$$\left(\frac{\partial e_{21}}{\partial v_2}\right)_T - \left(\frac{\partial e_{12}}{\partial v_1}\right)_T = -\left(\frac{\partial e_{23}}{\partial v_2}\right)_T + \left(\frac{\partial e_{32}}{\partial v_3}\right)_T = D. \quad (28)$$

Then we can subtract the second thermodynamic descriptivity condition (25) from the first one (24)

$$\left(\frac{\partial u_1}{\partial v_1}\right)_T - \left(\frac{\partial u_3}{\partial v_3}\right)_T = 2D. \quad (29)$$

The subtract can be interpreted as the total external action relative to system 2, which results in the influence of systems 1 and 3, simultaneously. Therefore, the magnitude of each action is the following:

$$D = \frac{1}{2} \left[\left(\frac{\partial u_1}{\partial v_1}\right)_T - \left(\frac{\partial u_3}{\partial v_3}\right)_T \right]. \quad (30)$$

Then we can represent the thermodynamic descriptivity conditions in terms of the states of neighbouring systems only

$$\begin{aligned} \left(\frac{\partial u_2}{\partial v_2}\right)_T &= \left(\frac{\partial u_1}{\partial v_1}\right)_T - \frac{1}{2} \left[\left(\frac{\partial u_1}{\partial v_1}\right)_T - \left(\frac{\partial u_3}{\partial v_3}\right)_T \right] = \\ &= \left(\frac{\partial u_3}{\partial v_3}\right)_T + \frac{1}{2} \left[\left(\frac{\partial u_1}{\partial v_1}\right)_T - \left(\frac{\partial u_3}{\partial v_3}\right)_T \right]. \end{aligned} \quad (31)$$

Thus, now we have a method for the calculation of the state of the system if states of its neighbouring systems are known. It is the basis of the thermodynamic model of the heat conduction process in a continuum. This model does not contain any partial differential equations. Instead, it includes simple rules of the updating of the states of cells as in (31). Such a model is realized by means of the continuous cellular automata algorithm described below.

3. CONTINUOUS CELLULAR AUTOMATA ALGORITHM

To describe the algorithm, we consider the two-dimensional heat conduction problem, concerning point-wise heating of a rectangular domain.

We apply the cellular automata technique for the solution of the formulated problem. As it is known [10], a cellular automaton is spatial lattice of N cells, each of which is in a certain state at time t . Each cell follows the same rule of updating its state. The state of the cell at time $t + 1$ depends on its own state and the state of neighbouring cells at time t . The cellular automaton starts out with some initial configuration of cell states, and at each time step, the states of all cells in the lattice are simultaneously updated.

In the heat conduction problem, we divide the domain into elements, each of which corresponds to a cell. Each element has the same size. We determine the state of each cell as the thermodynamic state of the corresponding element.

The essential feature of cellular automata is the rule of updating cell's states. Usually such a rule is expressed as a look-up table connecting the state of a cell with its local neighbourhood.

In our algorithm, we apply a generalization of the condition of local interaction between thermodynamic systems (31) as the rule of updating cell's states

$$\begin{aligned} \left(\frac{\partial u_{i,j}^{k+1}}{\partial v_{i,j}^{k+1}}\right)_T &= \\ &= \frac{1}{4} \left[\left(\frac{\partial u_{i-1,j}^k}{\partial v_{i-1,j}^k}\right)_T + \left(\frac{\partial u_{i+1,j}^k}{\partial v_{i+1,j}^k}\right)_T + \left(\frac{\partial u_{i,j-1}^k}{\partial v_{i,j-1}^k}\right)_T + \left(\frac{\partial u_{i,j+1}^k}{\partial v_{i,j+1}^k}\right)_T \right]. \end{aligned} \quad (32)$$

In the case of solids, mechanical properties are determined usually by means of the Young's modulus G , and Poisson's ratio ν . Thermal properties are taken into account by thermal expansion coefficient α . Generally speaking, all properties of solids depend on temperature. However, in the first approximation, we can consider them as uniform, as treated in many applications.

From the thermodynamical point of view, it is more convenient to use the bulk modulus K ,

$$K = \frac{G}{3(1 - 2\nu)} \quad (33)$$

because it has the clear thermodynamical meaning, namely,

$$K = -v \left(\frac{\partial p}{\partial v} \right)_T, \quad (34)$$

where v is the specific volume, p is pressure, T is temperature. The thermal expansion is expressed in thermodynamical terms as well

$$\alpha = \frac{1}{v} \left(\frac{\partial v}{\partial T} \right)_p. \quad (35)$$

The product of bulk modulus and thermal expansion coefficient determines another thermodynamic derivative

$$\alpha K = -v \left(\frac{\partial p}{\partial v} \right)_T \frac{1}{v} \left(\frac{\partial v}{\partial T} \right)_p = \left(\frac{\partial p}{\partial T} \right)_v, \quad (36)$$

which is immediately contained in the thermodynamic descriptivity condition (31) in view of (23). The assumption about the uniformity of thermal properties simplifies the rule of updating cell's states (32) in this case

$$4\alpha_{i,j}^k K_{i,j}^k T_{i,j}^k = \alpha_{i-1,j}^{k-1} K_{i-1,j}^{k-1} T_{i-1,j}^{k-1} + \alpha_{i+1,j}^{k-1} K_{i+1,j}^{k-1} T_{i+1,j}^{k-1} + \alpha_{i,j-1}^{k-1} K_{i,j-1}^{k-1} T_{i,j-1}^{k-1} + \alpha_{i,j+1}^{k-1} K_{i,j+1}^{k-1} T_{i,j+1}^{k-1}. \quad (37)$$

In the case of homogeneous medium, all elements have the same thermomechanical properties, and the rule of updating of cell's states (37) becomes even simpler. The temperature of each element is determined as the arithmetical mean of its neighbour's temperatures at the previous time step

$$T_{i,j}^k = \frac{1}{4} \left(T_{i-1,j}^{k-1} + T_{i+1,j}^{k-1} + T_{i,j-1}^{k-1} + T_{i,j+1}^{k-1} \right), \quad (38)$$

and it is fully independent of the kind of material. The calculations were performed for the rectangular domain. The typical number of elements was 200.

4. RESULTS AND DISCUSSION

The initial situation is given by the values of temperatures in each cell. We suppose that in the initial situation all elements have the same temperature 300 K. In a moment, one of the element at the boundary gets another value of temperature (400 K) and holds it in time. This boundary is supposed to be thermally insulated

$$\frac{\partial T_{1,j}^k}{\partial n} = 0, \forall k. \quad (39)$$

Cells at other boundaries hold their initial values

$$T_{N,j}^k = T_{N,j}^0, \quad T_{i,1}^k = T_{i,1}^0, \quad T_{i,M}^k = T_{i,M}^0, \quad \forall k. \quad (40)$$

The results of calculations for early times are shown in Fig. 1. Here we can see the propagation of the temperature front into the medium. For a sufficiently long duration, the temperature distribution approaches the steady-state one (Fig. 2).

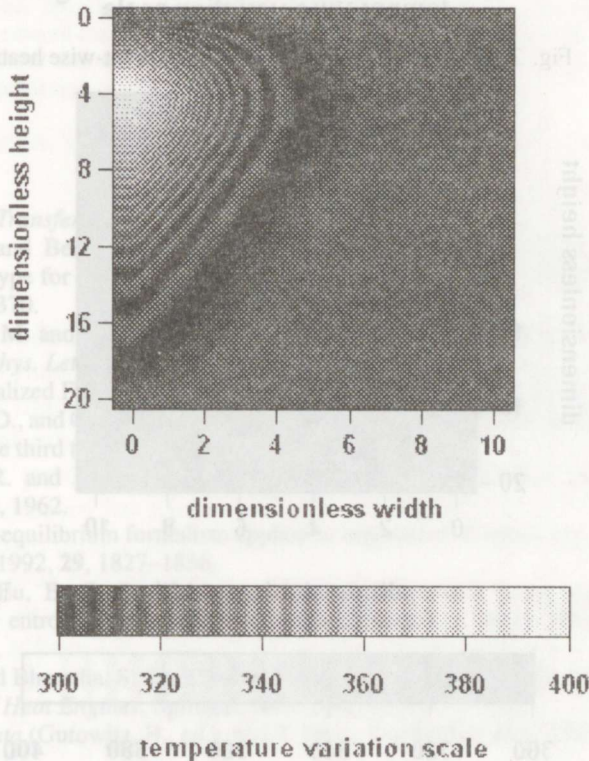


Fig. 1. Temperature distribution by point-wise heating at early times.

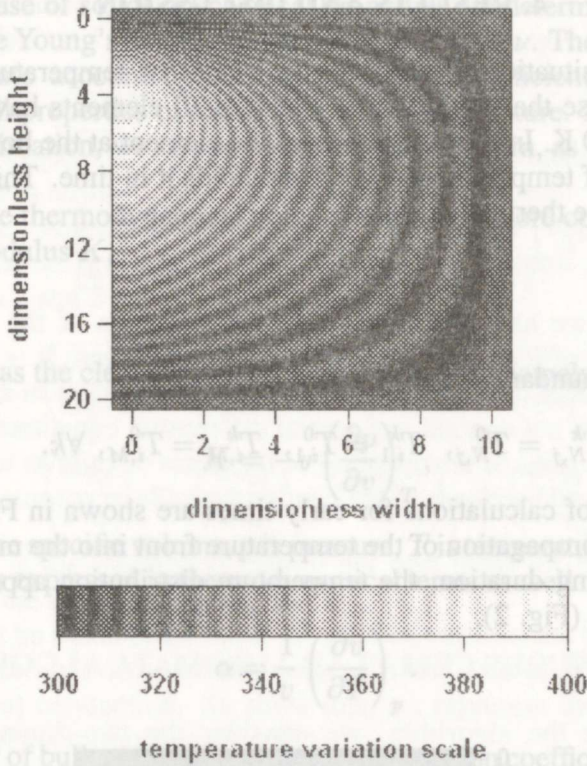


Fig. 2. Final temperature distribution by point-wise heating.

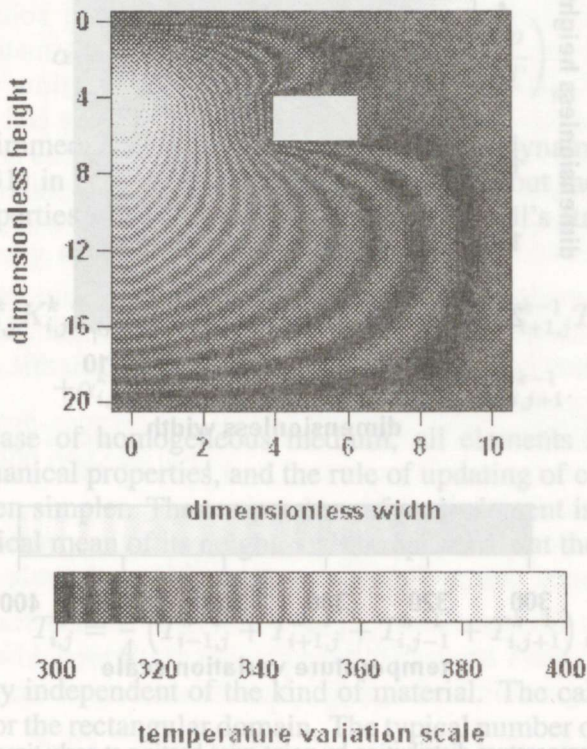


Fig. 3. Temperature distribution by point-wise heating in the case of more complicated geometry.

As an example of a more complex situation, we consider the same domain, from which some elements are removed. The created boundary keeps the initial temperature. As the calculation shows, in this case, the temperature distribution becomes more complicated (Fig. 3).

In conclusion, it should be noted that we had no need to solve any partial differential equations to determine the temperature distribution in the two-dimensional heat conduction problem. Consequently, the paradox of instantaneous propagation of thermal disturbances [4] was avoided.

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SOOJUSJUHTIVUSE TERMODÜNAAMILINE MODELLEERIMINE

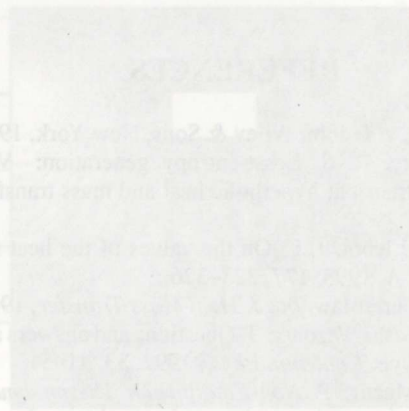
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Soojusjuhtivuse probleemide lahendamiseks on välja pakutud termodünaamiline lähenemisviis. Arvutusalgoritm baseerub ühelt poolt rakuautomaatide kasutamisel, teiselt poolt termodünaamika seadustel. Loakaalse tasakaalu hüpotees lubab pideva keskkonna iga elementi esitada homogeenne termodünaamilise süsteemina, mida võib käsitleda rakuna. Selliste rakkude oleku ruum on pidev, samal ajal kui tavaliselt vaadeldakse seda ruumi diskreetsena. Meetodi põhieelis seisneb diferentsiaalvõrrandite puudumises. Seetõttu on meetod pigem otseste protsesside modelleerimise vahend, aga mitte diferentsiaalvõrrandite lahendusmeetod. Rakendusnäitena on vaadeldud tahke keha kahemõõtmelist soojusjuhtivust.

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Fig. 2. Final temperature distribution by point-wise heating.



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Fig. 3. Temperature distribution by point-wise heating in the case of more complicated geometry.