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IMPROVEMENT OF THE METHOD OF CANONICAL ELEMENTS FOR MODELING TRANSFER PROCESSES IN SYSTEMS WITH CURVILINEAR BOUNDARIES

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The author discusses some methodological aspects of generalization and improvement of the accuracy of the method of canonical elements. Data of numerical experiments are compared to well-known exact analytical solutions of problems of heat transfer in regions with curvilinear boundaries.

Numerical modeling of heat transfer in solids of complicated geometry with curvilinear boundaries necessitates use of nonuniform difference grids. The method of finite elements [1], usually adopted for solution of such problems, has some disadvantages. The algorithm for its implementation is rather complicated and consumes much machine time. Estimation of the error in the results of solution by the method of finite elements involves certain difficulties. Moreover, it is strictly justified only for stationary problems.

In [2], a method of canonical elements for solids with curvilinear boundaries is described that is free of the above drawbacks. It consists in approximation of the transfer equation by the balance equation for a canonical element that is built on a nonuniform difference grid. Here, the derivatives along the coordinate axes are calculated as projections of the gradient of the sought function, which is determined by the values of this function at the nodes of the nonuniform grid.

The simplest difference grid for solids with curvilinear boundaries is the quasi-uniform grid, which for a two-dimensional singly connected region is as follows:

$$y_m = y' + m\Delta y, \quad m = 0, 1, \ldots, M, \quad y_M = y'';$$
$$x_{im} = x'_m + i\Delta x_m, \quad i = 0, 1, \ldots, I, \quad x_{Im} = x''_m; \tag{1}$$
$$\tau_n = n\Delta\tau, \quad n = 0, 1, \ldots, \quad \Delta\tau > 0,$$

where y' and y'' are the minimum and maximum values of the y coordinate for points of the region under consideration; x'_m and x''_m are the minimum and maximum values of the x coordinate for points on the coordinate line y_m. On this grid, a canonical element (rectangle) is determined by the coordinate lines $y_{m+1/2} = (y_m + y_{m+1})/2$, $y_{m-1/2} = (y_m + y_{m-1})/2$, $x_{i+1/2,m} = (x_{i+1,m} + x_{im})/2$, $x_{i-1/2,m} = (x_{im} + x_{i-1,m})/2$.

The heat fluxes q''_x and q'_x through the element faces $x_{i+1/2,m}$ and $x_{i-1/2,m}$ may be calculated by approximating the derivative of the sought temperature function t with respect to the x coordinate using central differences.

The heat fluxes q''_y and q'_y across the faces $y_{m+1/2}$ and $y_{m-1/2}$ are expressed by the derivatives of the function t with respect to the y coordinate, which are found as projections of the temperature gradient on this axis. The gradient is determined in terms of the derivatives of t with respect to x and some axis y' at the angle β_{yx} to the x axis, by the formula [2]

$$\frac{\partial t}{\partial y} = \frac{1}{\sin\beta_{yx}}\frac{\partial t}{\partial y'} - \mathrm{ctan}\,\beta_{yx}\frac{\partial t}{\partial x}. \tag{2}$$

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The heat flux q_y'' across the face $y_{m+1/2}$ may be calculated, in accordance with (2), by the difference equation

$$q_y'' = -\lambda \left\{ \frac{t^n_{j,m+1} + t^n_{im}}{y_{m+1} - y_m} - \left[\frac{t^n_{i+1,m} - t^n_{i-1,m}}{x_{i+1,m} - x_{i-1,m}} (1 - \theta_y) + \right. \right.$$
$$\left. \left. + \frac{t^n_{j+1,1,m+1} - t_{j-1,m+1}}{x_{j+1,m+1} - x_{j-1,m+1}} \theta_y \right] \frac{x_{i,m+1} - x_{im}}{y_{m+1} - y_m} \right\}, \quad 0 \le \theta_y \le 1 . \tag{3}$$

In [2], j is taken equal to i. Results of numerical experiments have shown that in order to improve the accuracy of the solution, it is expedient to choose j from the condition that the node (x_j, y_{m+1}) be at the minimum distance from the coordinate line x_i passing through the point (x_i, y_m), i.e., from

$$|r_{j,m+1} - r_{im}| = \min |r_{s,m+1} - r_{im}| , \quad s = 0, 1, \ldots, I . \tag{4}$$

The heat flux q_y' across the face $y_{m-1/2}$ is calculated by relations analogous to (3), (4).

In some cases, in using the method of canonical elements for regions of complicated configuration, it is necessary to determine the derivatives of the function t with respect to the x and y coordinates on the basis of its derivatives in the directions of some axes x' and y' that form the angles β_{xx} and β_{yx} with the x axis, respectively. Taking into consideration that the derivative of a scalar function in an arbitrary direction is equal to the projection of the gradient onto this direction, we write the following equations:

$$\frac{\partial t}{\partial x} = \cos \psi \operatorname{grad} t , \quad \frac{\partial t}{\partial x} = \sin \psi \operatorname{grad} t ,$$

$$\frac{\partial t}{\partial x'} = \cos (\psi + \beta_{xx}) \operatorname{grad} t , \quad \frac{\partial t}{\partial y'} = \cos (\beta_{yx} - \psi) \operatorname{grad} t ,$$

where ψ is the angle formed by the vector grad t and the x axis. Eliminating grad t and ψ from this system, we obtain formulas for calculating $\partial t/\partial x$ and $\partial t/\partial y$:

$$\frac{\partial t}{\partial x} = \left(\frac{1}{\sin \beta_{xx}} \frac{\partial t}{\partial x'} + \frac{1}{\sin \beta_{yx}} \frac{\partial t}{\partial y'} \right) \Big/ (\operatorname{ctan} \beta_{xx} + \operatorname{ctan} \beta_{yx}) , \tag{5}$$

$$\frac{\partial t}{\partial y} = \left(\frac{1}{\cos \beta_{yx}} \frac{\partial t}{\partial y'} + \frac{1}{\cos \beta_{xx}} \frac{\partial t}{\partial x'} \right) \Big/ (\tan \beta_{xx} + \tan \beta_{yx}) . \tag{6}$$

At $\beta_{xx} = 0$ formula (6) turns into (2), while (5) turns into the equality $\partial t/\partial x = \partial t/\partial x$. The mesh widths of the nonuniform difference grid may change within wide limits. Therefore, to improve the accuracy of a numerical solution it is useful to represent the three-layered explicit difference equation [3] in the following form:

$$c\rho \left[(1 + \theta_{im}) \frac{t^{n+1}_{im} - t^n_{im}}{\Delta\tau} - \theta_{im} \frac{t^n_{im} - t^{n-1}_{im}}{\Delta\tau} \right] = \frac{q_x' - q_x''}{\Delta x_m} + \frac{q_y' - q_y''}{\Delta y} , \quad \theta_{im} \ge 0 , \tag{7}$$

where the weight parameter θ is chosen dependent on the coordinates of the grid nodes. After choosing the mesh widths of the grid $\Delta\tau$, Δy, and Δx_m, the parameter θ_{im} is determined in conformity with the stability conditions for the difference equation (7) by the relation

$$\theta_{im} = \begin{cases} 0.5 \left(\dfrac{\Delta\tau}{\Delta\tau_{im}} - 1 \right) & \text{at} \quad \Delta\tau > \Delta\tau_{im} , \\ 0 & \text{at} \quad \Delta\tau \le \Delta\tau_{im} . \end{cases}$$

Here $\Delta\tau_{im}$ is the maximum step with respect to time corresponding to the two-layered explicit difference equation into which Eq. (7) turns at $\theta_{im} = 0$:

$$\Delta\tau_{im} = \frac{c\rho}{2\lambda}\left\{\left(\frac{x_{i+1,m} - x_{i-1,m}}{2}\right)^{-2} + \left(\frac{y_{m+1} - y_{m-1}}{2}\right)^{-2}\right\}.$$

Without a marked change in the error in the solution, the step $\Delta\tau$ may be chosen 5–7-fold greater than the minimum value of $\Delta\tau_{im}$.

Of importance in implementation of the method of canonical elements is approximation of the boundary conditions for heat transfer occurring under boundary conditions of the second and third kind. Let the heat transfer conditions at the boundary node (I, m) be

$$A\frac{\partial t}{\partial \nu} + Bt + C = 0\,, \tag{8}$$

where ν is the normal to the boundary surface.

The derivative $\partial t/\partial\nu$ may be determined in terms of the derivatives in the direction of the x coordinate and the direction of the tangent k to the boundary surface. Assuming $x = \nu$, $x' = x$, $y' = k$, $\beta_{yx} = \pi/2$, and $\beta_{xx} = (\widehat{\nu, x})$ in (3), we find

$$\frac{\partial t}{\partial \nu} = \frac{1}{\cos(\nu\,,\ x)}\frac{\partial t}{\partial x} + \tan(\nu\,,\ x)\frac{\partial t}{\partial k}\,. \tag{9}$$

In accordance with (9), Eq. (8) for the node $(x_{I,m}, y_m)$ is approximated by the equation

$$A\left[\frac{1}{\cos(\nu\,,\ x)}\frac{t_{I,m}^{n+1} - t_{I-1,m}^{n+1}}{x_{I,m} - x_{I-1,m}} + \tan(\nu\,,\ x)\times\right.$$

$$\left.\times\frac{(t_{I,m+1}^{n} - t_{I,m}^{n})\,h_{\bar{k}}^{2} + (t_{Im}^{n} - t_{I-1,m}^{n})\,h_k}{h_k h_{\bar{k}}\,(h_k + h_{\bar{k}})}\right] + Bt_{Im}^{n+1} + C = 0\,,$$

where h_k and $h_{\bar{k}}$ are the projections of the line segments connecting the point (x_{Im}, y_m) with the points $(x_{I,m+1}, y_{m+1})$ and $(x_{I,m-1}, y_{m-1})$, respectively, on the tangent to the boundary surface at the point (x_I, y_m).

In the absence of an analytical expression for the boundary surface the direction of the normal ν and tangent k at the point (x_{Im}, y_m) may be determined by the equation for the parabola passing through the points (x_{Im}, y_m), $(x_{I,m+1}, y_{m+1})$, and $(x_{I,m-1}, y_{m-1})$. For the quasi-uniform grid,

$$\operatorname{ctan}(k\,,\ x) = \frac{x_{I,m+1} - x_{I,m-1}}{2\Delta y}\,,\qquad \tan(\nu\,,\ x) = -\operatorname{ctan}(k\,,\ x)\,.$$

The method of canonical elements has been used to solve some problems of heat and mass transfer in bodies with curvilinear boundaries. To demonstrate the accuracy of the method, we present results of a comparison of numerical and well-known exact analytical solutions for unbounded solid and hollow cylinders. The numerical solution of axisymmetric heat transfer problems is accomplished in Cartesian coordinates (x, y) for 1/4 of the cylinder cross section. The difference grid is the union of nodes of the quasi-uniform grid:

$$y_m = m\Delta y\,,\quad m = 0\,,\ 1\,,\ \ldots\,,\ M\,,\quad \Delta y = R/M\,;\quad x_{im} = x'_m + i\Delta x_m\,,$$

$$i = 0\,,\ 1\,,\ \ldots\,,\ I\,,\quad \Delta x_m = (x''_m - x'_m)/(I-1)\,,\quad x'_m = R_{\text{in}}\sqrt{1 - (y_m/R_{\text{in}})^2}\,,$$

$$x''_m = R\sqrt{1 - (y_m/R)^2}\,;\quad \tau_n = n\Delta\tau\,,\quad n = 0\,,\ 1\,,\ \ldots\,,\quad \Delta\tau = \text{const} > 0$$

TABLE 1. Comparison of Numerical ($t(x, y)$) and Analytical ($t_a(r)$) Solutions of the Heat Conduction Problem in Unbounded Solid and Hollow Cylinders for Different Kinds of Boundary Conditions (KBC)

t	KBC	Fourier number						
		0.05	0.1	0.2	0.4	0.6	0.8	1.0
				Solid cylinder				
$t(0, 0)$	I	0.0139	0.1508	0.4970	0.8409	0.9500	0.9842	0.9951
$t_a(0)$	I	0.0183	0.1516	0.4985	0.8415	0.9501	0.9843	0.9951
$t(0, R/2)$	I	0.1636	0.3871	0.6607	0.8934	0.9664	0.9895	0.9966
$t(R/2, o)$	I	0.1645	0.3866	0.6613	0.8936	0.9665	0.9895	0.9966
$t_a(R/2)$	I	0.1644	0.3897	0.6620	0.8938	0.9666	0.9895	0.9966
$t(0, 0)$	II	0.0009	0.0243	0.1605	0.5387	0.9346	1.3315	1.7283
$t_a(0)$	II	0.000	0.026	0.168	0.517	0.9391	1.3466	1.7489
$t(0, R)$	II	0.2787	0.4063	0.6282	1.0315	1.4287	1.8256	2.2224
$t(R, 0)$	II	0.2705	0.4028	0.6235	1.0273	1.4247	1.8216	2.2184
$t_a(R)$	II	0.271	0.415	0.64	1.0358	1.4392	1.8466	2.236
$t(0, 0)$	III	0.0003	0.0215	0.1251	0.2508	0.5253	0.6532	0.7466
$t_a(0)$	III	0.00	0.024	0.132	0.35	0.53	0.66	0.75
$t(0, R)$	III	0.0217	0.304	0.4187	0.5779	0.6917	0.7747	0.8354
$t(R, 0)$	III	0.0222	0.3058	0.4160	0.5762	0.6905	0.7738	0.8348
$t_a(R)$	III	0.023	0.315	0.429	0.584	0.70	0.78	0.84
				Hollow cylinder, $\overline{R} = (R_{in} + R)/2$				
$t(0, R)$	I	0.5301	0.5672	0.5676	0.5676	0.5677	0.5678	0.5679
$t(\overline{R}, 0)$	I	0.5308	0.5776	0.5811	0.5811	0.5817	0.5818	0.5818
$t_a(\overline{R})$	I	0.525	0.562	0.5688	0.5688	0.5629	0.563	0.563

(R_{in} and R are the radii of the inner and outer surface of the infinite hollow cylinder) and nodes that lie at the intersection of the arc of a circle cut off by the coordinate line (chord) y_{M-1} and the coordinate lines $s_{i,M-1}$, $i = 0, 1, ..., I - 1$.

Table 1 presents results of solution of the heat conduction problem for an unbounded cylinder that has the constant temperature $t(0, r)$, $0 \le r \le R$ at the initial moment of time under boundary conditions of the first kind $t(\tau, R) = 1$, of the second kind at the Kirpichev number Ki = 1, and of the third kind at the Biot number Bi = 1 as well as for a hollow cylinder with $R_{in} = 0.5$ and boundary conditions of the first kind $t(\tau, R_{in}) = 0$, $t(\tau, R) = 1$.

A comparison of results of numerical determination of the temperature function at characteristic points of the considered region of space at $I = M = 17$ with values of the temperature t_a obtained for the same points of the region from exact analytical solutions [4] shows that the deviation of the solutions for the solid cylinder is, as a rule, within 1%, and for the hollow cylinder within 2%. It may be inferred that the error in modeling heat transfer by the method of canonical elements on nonuniform grids is close to that on uniform grids.

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