A. N. Khomchenko

UDC 536.2:518.12

A natural discretization scheme based on hexagonal finite elements is proposed for the numerical modeling of the temperature fields of honeycomb stuctures.

Schemes of the finite-element method (FEM), which are usually used in temperature-field calculations, are based on triangular and tetragonal finite elements (FE-3 and FE-4). The computational possibilities and approximational quality of these elements have been well studied and tested in numerous calculations [1-3]. In most cases, FE-3 and FE-4 are practical and effective. However, there are problems in which hexagonal elements (FE-6) are more convenient and useful. These include structures with a fundamental structural division into regular hexagons: honeycomb structures, nuclear-reactor lattices, etc. In discretizing a region, hexagons may be divided into triangles (as is often done), but the direct FE-6 construction is preferable, since this element, while ensuring sufficient accuracy, markedly reduces the volume of calculations. The discussion of modeling and the application of FE-6 is an urgent problem in light of the increasing interest of researchers in computational schemes with hexagonal cells.

The plane region Ω is divided into a series of nonoverlapping subregions or elements: $\Omega_1, \Omega_2, \ldots, \Omega_m, \ldots, \Omega_M$, where Ω_m is a regular hexagon with vertices 1, 2, ..., 6. All the elements interact through vertex-nodes 1, 2, ..., N. The generalized harmonic equation is written in the following form for a single element [4]

$$\frac{\partial}{\partial x}\left(h\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(h\frac{\partial u}{\partial y}\right)+\lambda u=p, \quad (x, y)\in\Omega_m,$$
(1)

with the boundary conditions

$$u = \tilde{u}$$
 on S_1 , $h \frac{\partial u}{\partial n} = q$ on S_2 .

At each FE-6, the function $\hat{u}(x, y)$ is formed by interpolating u(x, y) with respect to the vertices Ω_m . Piecewise interpolation is determined by the equation $\hat{u}(x, y) = u_m(x, y)$, $(x, y) \in \Omega_m$. The basis for determining $u_m(x, y)$ consists of the local functions $\phi_1, \phi_2, \ldots, \phi_6$, associated with vertices 1, 2, ..., 6. This means that

$$u_m(x, y) = \sum_{k=1}^{6} u(x_k, y_k) \varphi_k(x, y), \qquad (2)$$

where the coordinates x_k , y_k correspond to vertex k in Ω_m . Applying the Bubnov-Galerkin procedure to Eq. (1) and distributing the elements over ensembles gives a system of resolving equations with block matrices A_1 , ..., A_m , ..., A_M :

$\begin{bmatrix} A_1 \\ \vdots \\ A_m \end{bmatrix}$	$\begin{bmatrix} u_{t} \\ u_{2} \\ \vdots \\ \vdots \end{bmatrix}$	=	р, р ₂	,
	u _N		p _N	

Ivano-Frankovskii Institute of Petroleum and Gas. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 52, No. 2, pp. 301-305, February, 1987. Original article submitted February 26, 1986. where

$$A_{m} = K_{m} - \lambda M_{m}, \quad K_{m} = \int_{\Omega_{m}}^{\Omega} h \left(\Phi_{x}^{T} \Phi_{x} + \Phi_{y}^{T} \Phi_{y} \right) d\Omega,$$
$$M_{m} = \int_{\Omega_{m}}^{\Omega} \Phi^{T} \Phi d\Omega, \quad P_{m} = -\int_{\Omega_{m}}^{\Omega} p \Phi^{T} d\Omega + \int_{S_{x}}^{\Omega} q \Phi^{T} dS.$$

Note that the matrices K_m and M_m are symmetric, and the row matrix $\Phi = (\phi_1, \phi_2, \ldots, \phi_N)$ consists of basis functions.

Construction of the basis is a key point in FE modeling. Consider this procedure for FE-6. Suppose that the FE-6 nodes are at the vertices (Fig. 1). The traditional method [1, 2] of constructing the basis is to determine, for each vertex k, a six-parameter polynomial $\varphi_k(x, y) = \alpha_1 x^2 + \alpha_2 xy + \alpha_5 y^2 + \alpha_4 x + \alpha_5 y + \alpha_6$, solving the interpolation problem at hexagon $\varphi_k(x_k, y_k) = \delta_{kk}$ ($\ell = 1, 2, \ldots, 6$). The parameters α_1 are determined in terms of node values. Remembering that the basis function is 1 at "its" vertex, and vanishes at others, the following expression is written for k = 1:

$$\alpha_1 x_i^2 + \alpha_2 x_i y_i + \alpha_3 y_i^2 + \alpha_4 x_i + \alpha_5 y_i + \alpha_6 = \delta_{i1},$$

where i = 1, 6. The system obtained, however, does not have a solution, since its matrix is degenerate. This "singularity paradox" of FE-6 is associated with the axial symmetry of vertices of the element. There are various means of overcoming this deficiency of the traditional approach. The most effective and interesting new methods are those which eliminate the need to write and solve cumbersome systems of matrix-algebra equations. For example, local FE-6 basis functions may be constructed by means of the R-function method [5, 6]. An analogous approach was described in [7-9].

Consider a method of simplified construction of the FE-6 basis. Suppose that Ω_m is a regular hexagon of unit side (the vertex numbers are circled in Fig. 1). Begin with node 1. In constructing the function $\phi_1(x, y)$, use is made of a composition of the equations of sides 2-3, 3-4, 4-5, and 5-6 such that this function vanishes at the points 2, 3, ..., 6. The equation $\phi_1(x_1, y_1) = 1$ is attained by choice of an appropriate factor. The result obtained is

$$\varphi_1(x, y) = \frac{1}{4} \left(1 - \frac{4y^2}{3} \right) \left[(1+x)^2 - \frac{y^2}{3} \right].$$

The other functions of the basis are obtained from $\phi_1(x, y)$ by successive 60° rotation. The functions obtained, unlike the ordinary functions, do not satisfy the condition

$$\sum_{k=1}^{6} \varphi_k(x, y) = 1$$
 (3)

ensuring interelement continuity. This deficiency of the basis is eliminated by normalization using an appropriate functional factor, which leads to a piecewise-rational function

$$\varphi_1(x, y) = \left(1 - \frac{4y^2}{3}\right) \left[(1 + x)^2 - \frac{y^2}{3} \right] [2(3 - x^2 - y^2)]^{-1}$$

Note that the more complex structure of the normalized functions hinders the calculation of double integrals by FE-6 and this is not the only shortcoming of the piecewise-rational basis (PRB). An alternative to PRB is a polynomial basis (PB) constructed by an analogous method using a different composition of the lines passing through the FE-6 nodes. In this case, a quadratic parabola passing through nodes 2-4-6 and a straight line 3-5 is used in constructing $\phi_1(x, y)$. In contrast to PRB, the PB functions are normalized by means of a constant factor. The result obtained is

$$\varphi_1(x, y) = \frac{1}{6}(x-2y^2+1)(2x+1).$$



Fig. 1. FE-6 geometry and points of interpolation: the points of interpolation are circled; 0 (center of hexagon), 1, ..., 12 are points of integration.

Fig. 2. Computational FE-6 isotherms: dashed curves) PRB approximation; continuous curves) PB approximation.

The other PB functions are obtained from $\phi_1(\mathbf{x}, \mathbf{y})$ by 60° rotation. Note that, despite the satisfaction of Eq. (3) at any point of FE-6, the PB has specific differences from PRB. Thus, whereas for PRB the behavior of the function in Eq. (2) on a side of FE-6 is determined solely by the two basis functions associated with this side, for PB all the basis functions make a nontrivial contribution to the behavior of this function on the side of FE-6. An individual PB function manifests (although very weakly) some unusual properties: for example, nonlinearity on the sides adjacent to "its" vertex and nonzero values on the opposite FE sides. However, the properties of the individual function do not have undesirable consequences, since the mutually correcting influence of the basis functions completely eliminates any anomalies in the interpolated function. Thus, the two bases ensure C° smoothness on a hexagonal lattice.

As already noted, integration by FE-6 is a sufficiently complex and difficult operation. The computational procedure of [4] specially developed for "honeycomb" geometry is unsuitable for PRB. In this case, the Romberg integration method, based on Richardson extrapolation, must be used [4]. Completely satisfactory results of integration are obtained for both PB and PRB by means of a convenient 13-point quadrature formula specially constructed for FE-6

$$\iint_{\Omega} f(x, y) d\Omega = \max \Omega \left\{ \frac{1}{3} f(x_0, y_0) + \frac{5}{72} \sum_{i=1}^{6} f(x_i, y_i) + \frac{1}{24} \sum_{i=7}^{12} f(x_i, y_i) \right\},$$
(4)

where the points of integration are chosen at the center (a), at the vertices (b), and in the middle of the sides (c) of the inscribed hexagon (Fig. 1).

Special test examples are considered to compare the interpolation quality of PB and PRB. Thus, in the problem of node-by-node localization of the heat generated in FE-6 by an internal source, accurate calculation of the integrals is accompanied by approximate calculation by Eq. (4). As would be expected, the node fractions are 1/6, regardless of the type of basis; the results of accurate and approximate integration are the same. It is interesting to compare the FE-6 temperature fields modeled on the basis of PRB and PB. Suppose that constant temperatures of 120 and 0°C are maintained on sides 2-3 and 5-6, respectively, and a temperature of 60°C at points 1 and 4. Calculations show that the temperature distributions along the FE-6 boundaries are the same. However, inside the elements the temperature fields are not the same. These differences are illustrated by the calculational isotherms in Fig.2. There are grounds to suppose that the distorted PB isotherms are more correct. The dashed (PRB) isotherms do not reflect the FE-6 geometry, instead resembling the temperature field of tetragonal. Obviously, with increase in the number of sides of the polygon inscribed in the circle, the isotherms must tend to their limiting position, corresponding to the temperature field of a circular plate. Experience in using FEM shows that the passing to the limit does not always preserve the physical correctness of the solution obtained. It is enough to mention the

Sapondzhyan-Babushki paradox, which is well known in plate theory: in approximating a circular plate by means of regular polygons with freely supported edges, the limiting solution does not satisfy the conditions of free support at a circle [10].

In applying FEM, it is always important to remember the parasitic effects characteristic of the method: fictional solutions (nonphysical oscillations) and so-called engagement (an unreal increase in rigidity of the system). These effects largely affect the computational characteristics of FE and may distort seemingly ordinary calculations in the most unexpected manner. In this connection, it is difficult to overestimate the importance of preliminary testing of finite elements that have not been adequately studied.

NOTATION

u, temperature; h, thermal conductivity; p, internal-source (sink) function corresponding to an internal heat source (sink); λu , the same, but proportional to the temperature; \tilde{u} , temperature at boundary S_1 ; q, heat flux at boundary S_2 ; $S = S_1 + S_2$, total boundary of the region; $\partial u/\partial n$, derivative with respect to the normal at the boundary; δ_{ij} , Kronecker delta; mes Ω , measure (area) of FE-6; $f(x_i, y_i)$ value of integrand at point of integration i (i = 0, 1, 2, ..., 12).

LITERATURE CITED

- 1. E. Mitchell and R. White, Finite-Element Method for Partial Differential Equations [Russian translation], Moscow (1981).
- 2. O. K. Zenkevich, Finite-Element Method in Engineering [in Russian], Moscow (1975).
- 3. G. I. Marchuk and V. I. Agoshkov, Introduction to Projection-Grid Method [in Russian], Moscow (1981).
- 4. M. Ishiguro, I. Inf. Proc., 7, No. 2, 89-95 (1984).
- 5. V. L. Rvachev and A. P. Slesarenko, Logical Algebra and Integral Transformations in Boundary Problems [in Russian], Kiev (1976).
- 6. V. L. Rvachev and A. P. Slesarenko, Algebrological and Projectional Methods in Heat-Transfer Method [in Russian], Kiev (1978).
- 7. A. N. Khomchenko, Inzh.-Fiz. Zh., <u>49</u>, No. 2, 321-323 (1985).
- 8. A. N. Khomchenko, Resistance of Materials and Theory of Buildings [in Russian], Kiev (1980), No. 47, pp. 67-70.
- 9. L. I. Kamaeva and A. N. Khomchenko, in: Applied Strength Problems in Plasticity. Algorithmization and Automation of the Solution of Elasticity and Plasticity Problems. All-Union Intercollege Collection [in Russian], Gor'k. Gos. Univ. (1985), pp. 14-17.
- 10. V. G. Maz'ya and S. A. Nazarov, Dokl. Akad. Nauk ArmSSR, 78, No. 3, 127-130 (1984).