Features of the software implementation of the numerical solution of stationary heat equation taking into account the effects of nonlocal finite element method

G N Kuvyrkin, I Yu Savelyeva, A A Sokolov
Bauman Moscow State Technical University, 2nd Baumanskaya St., 5, building 1, Moscow, 105005
E-mail: fn2@bmstu.ru

Abstract. The features of the numerical solution of the two-dimensional equation of stationary heat conduction are considered taking into account nonlocal effects. The finite element method using isoparametric finite elements was chosen as the numerical solution scheme. A method for approximating the zone of nonlocal influence was proposed, and an estimate of the time for calculating the coefficients of the thermal conductivity matrix was also constructed. The influence of the main parameters of the model on the final results is studied, and a polynomial family of functions of non-local influence is also studied. The results are compared with the results obtained with the classical approach.

1. Introduction
Modern machinery provides high demands on the physical, mechanical and thermal properties of materials. Consolidated structurally sensitive materials possess these properties, which are obtained by compaction of nanopowders, deposition on a substrate, crystallization of amorphous alloys, and other methods [1–3].

To describe the behavior and properties of such materials, it is necessary to develop new mathematical models [4–6]. This is due to the fact that when considering micro- and nano-structured materials, classical approaches to continuum mechanics cease to work. This is due to the fact that effects begin to prevail in bodies of such sizes that do not significantly affect large bodies [7].

In this paper, we consider a model of stationary thermal conductivity taking into account nonlocal effects. The model is based on the approaches of generalized continuum mechanics. Moreover, the behavior of the material is described in such a way that the state of each particle of the body will depend on the state of all particles in this body [7, 8]. The main relations are presented in integro-differential form, which allows the use of well-studied numerical methods of solution. Such a technique for spreading the views of classical continuum mechanics on a medium with a micro- and nanostructure is called the continuous approximation method [9, 10].

In this paper, the search for a solution is carried out by the finite element method. The software implementation includes the use of sparse matrices taking into account their symmetry,
as well as the possibility of parallel assembly of the thermal conductivity matrix using OpenMP technology [11].

2. Mathematical model

In an arbitrary closed region \( S \subset \mathbb{R}^2 \) with a piecewise smooth boundary \( \partial S \) the equation of stationary heat conduction has the form [12]

\[
\nabla \cdot q = \lambda \nabla T + p_1 \sum_{e=1}^{N_e} \int_{S^e} \varphi(|x - x'|) \nabla x' T dS'(x'),
\]

where \( \nabla = \partial / \partial x_i e_i \) — is the nabla; \( e_i, \ i = 1, 2 \) — the unit vectors of coordinate axes; \( x_i, \ i = 1, 2 \) — the vector of components \( x \); \( q \) — the volumetric power density of internal sources and sinks of heat; \( q \) — the heat flux density vector, which is defined as follows [3, 4]

\[
q = \begin{cases}
\lambda \nabla T & \text{if } x' \in S^e(\mathbf{x}) \\
p_1 \sum_{e=1}^{N_e} \int_{S^e} \varphi(|x - x'|) \nabla x' T dS'(x') & \text{otherwise}
\end{cases}
\]

where \( \lambda \) — the coefficient of thermal conductivity; \( p_1 > 0 \); \( p_2 > 0 \) — the nonlocality (weight) parameters such that \( p_1 + p_2 = 1 \); \( \varphi \) — the nonlocal influence function, some normalized positive function in the region \( S^e(\mathbf{x}) \); \( S^e(\mathbf{x}) \) — the nonlocal area of influence; \( x' \in S^e(\mathbf{x}) \).

The term containing in the weight factor \( p_1 \) in (2) corresponds to the classical concept of heat transfer in the body (the Biot — Fourier law of thermal conductivity) [9]. The integral term, with the weight factor \( p_2 \), describes the effect of the nonlocal influence of points in the region \( S^e(\mathbf{x}) \) on the point \( \mathbf{x} \) currently under consideration.

Consider the boundary conditions of the first and second kinds for an equation (1) of the following form

\[
T|_{\Gamma_1} = f(\mathbf{x}), \quad q \cdot n|_{\Gamma_2} = g(\mathbf{x}),
\]

where \( \Gamma_1, \Gamma_2 \subset \partial S \); \( \Gamma_1 \cup \Gamma_2 = \emptyset \); \( f(\mathbf{x}) \); \( g(\mathbf{x}) \) — some functions that specify the temperature and flow at the boundary, respectively.

Entry grid finite element model \( S_h \) on the area \( S \). Using standard finite element approach [13, 14] to the equation (1) and substitute it (2). Obtain the equation [15]

\[
\int_S \sum_{e=1}^{N_e} \frac{\partial N_i^{(e)}}{\partial x_k} \partial N_j^{(e)} dS + p_1 \sum_{e=1}^{N_e} \int_{S^e} \varphi(|x - x'|) \frac{\partial N_j^{(e)}}{\partial x_k} dS'(x') dS' = \mathcal{K}
\]

where \( \mathcal{K} \) — the i-th basic element function \( (e) \); \( T_j^{(e)} \) — the desired temperature value \( T \) on the element \( (e) \) in the j-th node; \( k, j = 1, M(e); j' = 1, M' e) \); \( (e) \in S_k; (e') \in S_h; M'(e') \) and \( M'(e') \) — the number of nodes of elements \( (e) \) and \( (e') \), respectively.

3. Choice of nonlocal influence function

For calculations, a family of polynomial functions with a limited radius of influence of the following form will be selected as functions of nonlocal influence

\[
\varphi_{p,q}(|x - x'|) = \begin{cases}
\frac{p}{2\pi r^2 B(2/p, q + 1)} \left( 1 - \left( \frac{|x - x'|}{r} \right)^p \right)^q, & |x - x'| \leq r, \\
0, & |x - x'| > r,
\end{cases}
\]
where \( p, q > 0, \ r > 0 \) is the radius of nonlocal influence, \( B \) is Euler beta function.

Varying the parameters \( p \) and \( q \) we can notice that as the parameter \( p \) increases, the distribution of the influence function becomes more uniform and in the limit we get the constant \((\pi r^2)^{-1}\), while as the parameter \( q \) increases, the distribution becomes more concentrated in the center of the region and in the limit we get the Dirac delta function, which will give us the classical Biot — Fourier law of thermal conductivity [9]. The graphs of the wagging functions in the section along the axis of symmetry for various parameters \( p \) and \( q \) are presented in figure 1 and figure 2.

4. Numerical solution
Zone nonlocal influence \( S'(x) \) approximated as follows. We calculate the centers of all the elements of the grid and for each we search for the nearest neighbors in the zone of a given radius relative to the center of the element. If the center of an adjacent element falls into the sphere of influence, it is accounted for in the calculation. Figure 1 shows a conditional portrait of an approximated zone of nonlocal influence for an element marked with a cross. The actual zone of influence is shown by a circle approximated grayed zone, the centers of elements marked by dots. When approximating the radius should be chosen somewhat greater than the actual
radius of the non-local influence. Thus, we guarantee that all quadrature nodes that fall into the zone of nonlocal influence of $S'(x)$ will participate in the calculation.

When calculating the left side of the equation (4), we obtain a symmetric thermal conductivity matrix, which is convenient to store in a sparse form. This matrix is much more filled than the classical formulation of the problem ($p_1 = 1$). RAM requirements in the problem grows quadratically with respect to the number of elements in a grid or radius nonlocal influence (in the classical formulation requirements linear growth).

Based on the time it takes to assemble the thermal conductivity of the matrix in the classical formulation, it is possible to build a time estimate it will take to build a matrix in a nonlocal statement on the same formula grid

$$t_{NonLocal} = MQ t_{Local},$$

where $t_{Local}$ $t_{NonLocal}$ — the time required to assemble the matrix in classical and nonlocal settings, respectively; $M$ — the average number of nearest neighbors; $Q$ — the average number of nodes of the quadrature. Based on this formula, the time required to calculate the coefficients of the thermal conductivity matrix in a nonlocal setting will increase quadratically with respect to the number of grid elements or the radius of nonlocal influence, since when the grid is crushed or the radius increases, the average number of neighbors for each element will quadratically increase.

5. Results

After considering specific examples, it is possible to ensure the rapid growth of requirements for RAM size and the time required for the calculation of the thermal conductivity coefficient matrix. Table 1 shows the results of calculations by quadratic serendipity elements at several uniform grids, entered on the unit square $S = [0, 1] \times [0, 1]$, at different radii nonlocal influence. When the mesh is crushed or when the radius of the non-local influence increases, a quadratic increase in the requirements of RAM and counting time is observed. It is also possible to ensure the health evaluation (5), taking over $M$ value from the table and $Q = 9$. It is important that this time estimate was obtained taking into account pre-calculated Jacobi matrices for all quadrature grid nodes. The algorithm is amenable to parallelization good.
Table 1. Requirements of RAM volumes and the speed of calculating the coefficients of the thermal conductivity matrix in serial and parallel modes on different grids with different radii of non-local influence.

| Qty elements | Radius influences | Average qty neighbors | Volume memory, Mb | Counting time, s (1 thread) | Counting time, s (4 threads) |
|--------------|-------------------|-----------------------|------------------|----------------------------|----------------------------|
| 2500         | 0                 | —                     | 1                | 0.027                      |                            |
| 2500         | 0.1               | 67                    | 17               | 14                         | 3.6                        |
| 2500         | 0.2               | 259                   | 55               | 57                         | 14                         |
| 10000        | 0                 | —                     | 4                | 0.11                       |                            |
| 10000        | 0.1               | 284                   | 243              | 252                        | 65                         |
| 10000        | 0.2               | 1050                  | 824              | 948                        | 243                        |

To demonstrate the performance of the algorithm, the next problem will be considered. In the region $S = [0, 1] \times [0, 1]$ the mesh $S_h$ of 10000 bilinear elements is introduced. The boundary conditions are written as

$$T|_{x_2=0} = 0, \quad T|_{x_2=1} = 1, \quad q \cdot n|_{0<x_2<1} = 0.$$  

In the classical setting, that is, for $p_1 = 1$, the solution is the plane $T(x) = x_2$, but when non-local effects are taken into account, the solution is a more complex surface. Figure 4 shows the differences of solutions taking into account nonlocal effects and without in various sections. It can be noted that, when approaching the boundaries, the deviations increase, while in the center of the region they are absent. This phenomenon is explained by the fact that, at the boundary, the influence of the classical Biot — Fourier law [9] increases, since the nonlocal influence zone $S'(x)$ is cut off by the boundary $\partial S$ and the contribution of the integral term decreases.

![Figure 4](image-url)

Figure 4. The difference of solutions in nonlocal and local settings in different sections.

Using the same problem as an example, we will study the influence of the main parameters of the model on the final results. With an increase in the contribution of non-local influence, that is, with a decrease in the parameter $p_1$, the deviations become larger. With an increase in the radius of nonlocal influence $r$, the deviation also increases. The calculation results are shown in figure 5 and 6.
Next, we consider the Neumann problem on the same region $S$, with the mesh $S_h$ introduced on it. We set the boundary conditions

$$q \cdot n|_{x_2=0} = -1, \quad q \cdot n|_{x_2=1} = 1, \quad q \cdot n|_{0<x_2<1} = 0.$$ 

This problem has infinitely many solutions that differ by a constant, therefore, to obtain a specific solution, we put an additional condition

$$\int_S T d\mathbf{x} = 0.$$ 

Using the example of this problem, we compare the solutions obtained in the classical and nonlocal formulations with various influence functions.

The difference between the solutions in the nonlocal and classical settings is illustrated in figure 7. It can be noted that as the parameter $p$ increases, the divergence of solutions becomes larger and tends to the solution when the influence function is equal to the constant $(\pi r^2)^{-1}$. During integration (4), quadratures were chosen that can accurately calculate polynomials of given degrees.

As the parameter $q$ increases, the differences between the classical and nonlocal approaches become smaller. This is clearly illustrated in figure 8.
Next we consider the T-shaped region $S$ shown in figure 9, with a uniform grid of 7500 $S_h$ elements introduced on it. Set the boundary conditions

$$T|_{x_2=0} = 0, \quad T|_{x_2=1} = 1, \quad q \cdot n|_{0<x_2<1} = 0.$$

Figures 9 and 10 show the level lines of the solutions of the equation (1) for various weight parameters $p_1$. Figure 9 shows that when approaching the upper and lower boundaries, there is a discrepancy between the classical solution and the solution taking into account nonlocal effects. The greater the contribution of nonlocal influence, the greater the difference. The greatest deviations are observed in the vicinity of the central corners. A more detailed consideration of the subdomain $S_1 = [0.25, 0.5] \times [0.4, 0.5]$ makes it clear that the level lines of solutions that take into account nonlocal effects noticeably change their character when approaching the boundaries. Inside the region, their character is similar to the classic, but with some discrepancies. This fact is well shown in Figure 10. A characteristic feature of solutions that take into account nonlocal effects is that the level lines enter the boundary not at right angles. The calculated parameters and the nature of the lines that correspond to them are indicated in the figures.
Figure 9. Distribution of level lines in the T-shaped region.

Figure 10. Subregion $S_1$ in the T-shaped region.
We also consider the Neumann problem on a T-shaped domain. We set the boundary and additional conditions

\[ q \cdot n|_{x_2=0} = \pm 2, \quad q \cdot n|_{x_2=1} = \mp 1, \quad q \cdot n|_{0<x_2<1} = 0, \]
\[ \int_S T \, dx = 0. \]

Figure 11 shows the level lines of the solutions of the equation (1) with different weight parameters \( p_1 \). When changing the signs of flows at the boundaries \( x_2 = 0 \) and \( x_2 = 1 \) the level lines will also change their sign, but their character will remain the same. At the same time, we note that the intersection line of the solutions is a line very close to 0, which leaves the central nodes of the region. As in the problem with temperatures set on the same boundaries, strong discrepancies of the solutions are noticeable in the corners of the region for various weight parameters \( p_1 \).

\[ \text{Figure 11. Distribution of level lines in the T-shaped region in the Neumann problem.} \]

6. Conclusions
A two-dimensional stationary model of thermal conductivity taking into account nonlocal effects was considered. A solution algorithm based on the finite element model was implemented and a program was written in the C++ programming language. Parallelization of the thermal conductivity matrix assembly algorithm was performed using OpenMP technology. For storage and solution of sparse SLAEs, the Eigen library was used. An estimate of the assembly time of the thermal conductivity matrix was constructed. The effects of the main parameters of the model and various functions of nonlocal influence on the final results were analyzed.
Acknowledgments
The research was supported by the Russian Federation for Basic Research project No. 18-38-20108.

References
[1] Alymov M I and Zelensky V A 2005 Production methods and physicomechanical properties of bulk nanocrystalline materials (Moscow: Elise)
[2] Kuvyrkin G N and Savelyeva I Yu 2019 One mathematical model of heat conduction in nonlocal medium (College Park: AIP Conference Proceedings 2116, 380007)
[3] Kuvyrkin G N, Savelyeva I Yu and Zhuravsky A V 2018 Numerical Simulation of Vapor-Phase Epitaxy with Allowance for Diffusion Processes vol 10, issue 3 (Mathematical Models and Computer Simulations) pp 299–307.
[4] Zarubin V S, Kuvyrkin G N and Savelyeva I Yu 2011 Nonlocal mathematical model of thermal conductivity in solids vol 3 (Moscow: Bulletin of MSTU N E Bauman. Ser. Natural Sciences)
[5] Gopalakrishnan S and Narendar S 2013 Wave Propagation in Nanostructures. Nonlocal Continuum Mechanics Formulations (New York: Springer International Publishing) p 365
[6] Zarubin V S, Kuvyrkin G N and Savelyeva I Yu 2016 Evaluation of the Linear Thermal Expansion Coefficient of a Composite with Disperse Anisotropic Inclusions by the Self-Consistency Method vol 52, issue 2 (Riga: Mechanics of Composite Materials) pp 143–154
[7] Eringen A C 2002 Nonlocal continuum field theories (New York-Berlin-Heidelberg: Springer-Verlag) p 393
[8] Kuvyrkin G N and Savelyeva I Yu 2016 Thermomechanical model of nonlocal deformation of a solid vol 51, issue 3 (Moscow: Mechanics of Solids) pp 256–262
[9] Kunin I A 1975 Theory of elastic media with a microstructure. Nonlocal theory of elasticity (Moscow: The science) p 416
[10] Onami M, Iwashimizu S, Hauk K, Shiozawa K and Tanaka K 1987 Introduction to micromechanics (Moscow: Metallurgy) p 280
[11] Antonov A S 2009 Parallel programming using OpenMP technology (Moscow: Moscow University Press) p 78
[12] Zarubin, V S and Kuvyrkin G N 2008 Mathematical Models of Continuum Mechanics and Electrodynamics (Moscow: The Bauman University Publishing House) p 512
[13] Zienkiewicz O, Taylor R and Zhu J Z 2013 The Finite Element Method: Its Basis and Fundamentals. Seventh edition (Oxford: Butterworth-Heinemann) p 756
[14] Bathe K-J 2014 Finite Element Procedures. Second edition (Watertown) p 1065
[15] Kuvyrkin G N and Savelyeva I Yu 2014 Numerical solution of integro-differential heat conduction equation for a nonlocal medium (Moscow: Mathematical Models and Computer Simulations)