Numerical implementation of the Lame equation with complex boundary conditions

S B Sorokin\textsuperscript{1,4}, A G Maksimova\textsuperscript{1,3,4}, G G Lazareva\textsuperscript{1,2,4,5} and A S Arakcheev\textsuperscript{3,5}

\textsuperscript{1} Institute of Computational Mathematics and Mathematical Geophysics SB RAS 6, Ac. Lavrentieva Pr., Novosibirsk, 630090, Russian Federation

\textsuperscript{2} Peoples' Friendship University of Russia (RUDN University) 6, Miklukho-Maklaya str., Moscow, 117198, Russian Federation

\textsuperscript{3} Budker Institute of Nuclear Physics SB RAS 11, Ac. Lavrentieva Pr., Novosibirsk, 630090, Russian Federation

\textsuperscript{4} Novosibirsk State University 1, Pirogova str., Novosibirsk, 630090, Russian Federation

\textsuperscript{5} Novosibirsk State Technical University 20, Prospekt K. Marksa, Novosibirsk, 630073, Russian Federation

E-mail: sorokin@sscc.ru, maksimova@oapmg.sscc.ru, lazareva@ssd.sscc.ru, asarakcheev@gmail.com

Abstract. A discrete model is constructed for calculating the Lame equation with complex boundary conditions. The model is tested on an analytical solution. A complex boundary condition arises when a microcrack is specified on one of the boundaries. Calculation of microcracks will enable better assessment of the relevance of the simulation and finding out which mechanisms will occur in the case of plasma flow heating in modern plasma and future thermonuclear installations.

1. Introduction

One of the most critical problems in the international experimental thermonuclear reactor (ITER project) is design of first wall and divertor plates. Plates material should conduct heat well, spray a small amount of particles into plasma, accumulate little hydrogen and so on. These materials must not be destroyed mechanically, melt and spray out under action of the expected effects in a tokamak. Problems of durability of materials exposed to the high-power plasma streams relevant for fusion reactors on the basis of a different geometry of the magnetic field. Results on the heating of a tungsten plate by a pulsed electron beam were obtained on the experimental setup BETA (Beam of Electrons for materials Test Applications) at BINP SB RAS [1]. The full-scale experiment goes in parallel with computational ones [2]. The calculation of displacements around microcracks perpendicular to the surface is very relevant. The work is devoted to the numerical implementation of the Lame equation with complex boundary conditions. A complex boundary condition arises when a microcrack is specified on one of the boundaries. The aim of the study is to simulate the erosion of the sample surface as a result of evaporation and penetration of heat flux into the material taking into account microcracks [3].
2. Problem definition
Consider a mathematical two-dimensional model of the linear static theory of elasticity [4]. The model includes the equation of equilibrium, Hooke's law and relations "displacement-deformation":

\[
\begin{align*}
\text{div } \mathbf{\sigma} &= \mathbf{f}, \\
\mathbf{\sigma}_{ij} &= 2\mu \mathbf{\varepsilon}_{ij} + \lambda (\mathbf{\varepsilon}_{11} + \mathbf{\varepsilon}_{22}) \delta_{ij}, \quad i, j = 1, 2, \\
\mathbf{\varepsilon}_{ij} &= \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \quad i, j = 1, 2.
\end{align*}
\]

where \(\mathbf{\sigma}\) – is stress tensor with components \(\mathbf{\sigma}_{ij}\); \(\mathbf{f}\) – is mass force vector; \(\mu, \lambda\) – are Lame constants; \(\mathbf{\varepsilon}_{ij}\) – are components of the strain tensor \(\mathbf{\varepsilon}\); \(\delta_{ij}\) – is Kronecker symbol; \(u_i\) – are components of the displacement vector \(\mathbf{u}\).

As well as in [5, 6] we represent mathematical model in conjugate-operator form:
equation of equilibrium:

\[
R^* \mathbf{\sigma} = \mathbf{f},
\]

Hooke's law:

\[
\mathbf{\sigma} = K \mathbf{\varepsilon}, \quad \text{where } K = \begin{bmatrix}
\lambda + \mu & \lambda & 0 \\
\lambda & \lambda + \mu & 0 \\
0 & 0 & \mu
\end{bmatrix},
\]

and relations "displacement-deformation":

\[
\mathbf{\varepsilon} = R \mathbf{u} = \begin{bmatrix}
\frac{\partial}{\partial x_1} & 0 \\
0 & \frac{\partial}{\partial x_2} \\
\frac{\partial}{\partial x_2} & \frac{\partial}{\partial x_1}
\end{bmatrix} \mathbf{u}.
\]

The last three equations introduce vectors

\[
\mathbf{\sigma} = (\mathbf{\sigma}_{11}, \mathbf{\sigma}_{22}, \mathbf{\sigma}_{12})^T, \quad \mathbf{\varepsilon} = (\mathbf{\varepsilon}_{11}, \mathbf{\varepsilon}_{22}, 2\mathbf{\varepsilon}_{12})^T,
\]

composed of components of tensors \(\mathbf{\sigma}\) and \(\mathbf{\varepsilon}\).

To solve the problem, we will use the statement “in displacements”. We obtain the necessary equation for determining the displacements by substituting the expression for \(\mathbf{\varepsilon}\) from the "displacement-deformation" relation in Hooke's law, then we substitute the result into the equation of equilibrium. As a result, we get:

\[
R^* KR \mathbf{u} = \mathbf{f}.
\]

The main difficulty in discretization this problem is the construction of an approximation of the boundary conditions specified in terms of stresses. The need to preserve the basic properties of the operator of a differential problem at a discrete level requires cumbersome and far from obvious arguments. The discrete analogue construction scheme described in the next section is quite simple to implement and obviously leads to self-conjugate positive definite approximations of the static problem of the theory of elasticity in the formulation of “displacement”. In this case, the boundary conditions specified in terms of stresses are approximated automatically.
3. The difference scheme

The mathematical model of the problem of the theory of elasticity belongs to the class of models having a conjugate-operator structure [5, 6]. To maintain this structure at the difference level, the following procedure is used to construct a discrete analogue [6, 7]:

- The operator R is selected as the support.
- An approximation of \( R \) is constructed.
- The approximation of \( R^* \) conjugate to the selected operator is constructed as the operator conjugate to \( R \).

Consider a rectangular domain \( \Omega = [a, b] \times [c, d] \). We introduce two rectangular grids (Fig. 1):

\[
\bar{\Omega} = \{ x_{i,j} = (x_i, y_j) : x_i = a + ih_x, \quad i = 0, \ldots, N_x + 1, \\
y_j = c + jh_y, \quad j = 0, \ldots, N_y + 1, \\
\}
\]

\[
\Omega = \{ x_{i,j} = \left( x_{i}, y_{j} \right) : x_{i} = a + \left( i + \frac{1}{2} \right) h_x, \quad i = 0, \ldots, N_x, \\
y_{j} = c + \left( j + \frac{1}{2} \right) h_y, \quad j = 0, \ldots, N_y, \\
\}
\]

where \( h_x = \frac{b - a}{N_x + 1}, \quad h_y = \frac{d - c}{N_y + 1} \) - are space steps. The values of the displacement vector \( \mathbf{u} \) are determined at the nodes of the first grid. In the nodes of the second grid, the values of the strain tensor \( \mathbf{\varepsilon} \) and stress tensor \( \mathbf{\sigma} \) are determined.

![Figure 1. The grid scheme.](image)

We introduce:

- \( H_h \) - the Hilbert space of grid vector-functions \( \mathbf{u}^h = (u_1^h, \ldots, u_N^h)^T \) defined on the grid \( \bar{\Omega} \):

\[
\mathbf{u}^h(x_{i,j}) = \left( u_1^h(x_{i,j}), \ldots, u_N^h(x_{i,j}) \right)^T \equiv \mathbf{u}_{i,j}^h = \left( u_{i,j}^h, u_{i,j}^h \right)^T, \quad \text{with the scalar product:}
\]

\[
(\mathbf{u}^h, \mathbf{v}^h) = \sum_{i,j} u_{i,j}^h v_{i,j}^h h_x h_y
\]
\[(\mathbf{u}^h, \mathbf{v}^h)_{H^k} = \sum_{h_i \in \mathcal{H}} [u_i^h(x_{i,j})v_i^h(x_{i,j}) + u_i^h(x_{i,j})v_i^h(x_{i,j})] \hat{h}_{i,j}, \]

\[\forall \, \mathbf{u}^h \in H^k, \, \mathbf{v}^h \in H^k.\]

\[\hat{h}_{i,m} = \begin{cases} 0,5 \hat{h}_i, & m = 0, \\ 0,5 \hat{h}_i, & 1 \leq m \leq N_y, \\ 0,5 \hat{h}_i, & m = N_y + 1. \end{cases}\]

\[H^*_h \quad \text{is the Hilbert space of grid vector-functions } \sigma^h = (\sigma_{11}^h, \sigma_{22}^h, \sigma_{12}^h)^T \text{ defined on the grid } \omega \frac{1}{2}.\]

\[\sigma^h(x_{i, j}) = (\sigma_{11}^h(x_{i, j}), \sigma_{22}^h(x_{i, j}), \sigma_{12}^h(x_{i, j}))^T \equiv \sigma_i^h = (\sigma_{11}^h, \sigma_{22}^h, \sigma_{12}^h)^T,\]

with the scalar product:

\[(\mathbf{w}^h, \sigma^h)_{H^k} = \sum_{i, j=0 \frac{1}{2}}^N \left[ w_{i, j}^h(x_{i, j}) \sigma_{11}^h(x_{i, j}) + w_{i, j}^h(x_{i, j}) \sigma_{22}^h(x_{i, j}) + w_{i, j}^h(x_{i, j}) \sigma_{12}^h(x_{i, j}) \right] \hat{h}_{i,j}, \]

\[\forall \, \mathbf{w}^h \in H^*_h, \quad \sigma^h \in H^*_h.\]

To approximate \( R \), we will use the following operator \( R_h : H^k \rightarrow H^*_h \) [8]:

\[(R_h \mathbf{u}^h)_{i, j} = \frac{1}{2} \begin{bmatrix} \frac{u_{i+1, j}^h - u_{i, j}^h}{h_i} + \frac{u_{i+1, j+1}^h - u_{i, j+1}^h}{h_i} \\ \frac{u_{2, j+1}^h - u_{2, j}^h}{h_y} + \frac{u_{2, j+1}^h - u_{2, j+1}^h}{h_y} \\ \frac{u_{i+1, j+1}^h - u_{i+1, j}^h}{h_i} + \frac{u_{i+1, j}^h - u_{i+1, j+1}^h}{h_i} + \frac{u_{i, j+1}^h - u_{i, j}^h}{h_i} + \frac{u_{i, j+1}^h - u_{i, j+1}^h}{h_i} \end{bmatrix}.\]

The operator \( R_h^* \) was built as conjugate to \( R_h \), namely \( R_h^* = (R_h)^* : H^*_h \rightarrow H^k \)

\[(\mathbf{w}^h, R_h \mathbf{u}^h)_{H^*_h} = (R_h^* \mathbf{w}^h, \mathbf{u}^h)_{H^k}.\]

Using the summation formulas in parts, we obtain

\[R_h^* \mathbf{w}^h(x_{i,j}) = \frac{1}{2} \begin{bmatrix} \frac{w_{i+1, j+1}^h}{h_i} - \frac{w_{i+1, j}^h}{h_i} - \frac{w_{i, j+1}^h}{h_i} + \frac{w_{i, j}^h}{h_i} \\ \frac{w_{2, j}^h}{h_y} - \frac{w_{2, j+1}^h}{h_y} + \frac{w_{2, j+1}^h}{h_y} \frac{w_{2, j}^h}{h_y} \\ \frac{w_{i, j+1}^h}{h_i} - \frac{w_{i+1, j+1}^h}{h_i} + \frac{w_{i+1, j}^h}{h_i} + \frac{w_{i, j}^h}{h_i} \end{bmatrix}.\]

The resulting operator \( R_h^* \) can only be used to calculate values at internal nodes of the grid \((i = 1, \ldots N_x, j = 1, \ldots N_y)\). In this case, the scheme is applicable only if a displacement vector \( \mathbf{u} \) is specified at the boundary, which imposes significant restrictions on the statement of the problem.

For problems where the stress tensor \( \sigma \) is specified at some boundaries, the operator needs to be expanded. The following is an example for calculating at the boundary of the domain for \( i = 0 \):

\[R_h^* \mathbf{w}^h(x_{0,j}) = \frac{1}{2} \begin{bmatrix} \frac{w_{i+1, j+1}^h}{h_i} - \frac{w_{i+1, j}^h}{h_i} - \frac{w_{i, j+1}^h}{h_i} + \frac{w_{i, j}^h}{h_i} \\ \frac{w_{2, j}^h}{h_y} - \frac{w_{2, j+1}^h}{h_y} + \frac{w_{2, j+1}^h}{h_y} \frac{w_{2, j}^h}{h_y} \\ \frac{w_{i, j+1}^h}{h_i} - \frac{w_{i+1, j+1}^h}{h_i} + \frac{w_{i+1, j}^h}{h_i} + \frac{w_{i, j}^h}{h_i} \end{bmatrix} = \begin{bmatrix} \frac{-2}{h_i} \sigma_{11,0} - f_{1,0} \\ \frac{-2}{h_i} \sigma_{12,0} - f_{2,0} \end{bmatrix}.\]

Similar operators are introduced for all necessary boundaries.
An approximation of the boundary conditions specified in terms of stresses in the lower left corner of the computational domain is written as

\[
\begin{pmatrix}
-2 \frac{w_{11,1/2,1/2}}{h_x} & -2 \frac{w_{12,1/2,1/2}}{h_y} \\
-2 \frac{w_{12,1/2,1/2}}{h_y} & -2 \frac{w_{11,1/2,1/2}}{h_x}
\end{pmatrix} = 
\begin{pmatrix}
-2 \frac{\sigma_{11,0,1/2}}{h_x} - 2 \frac{\sigma_{12,1/2,0}}{h_x} - t_{x00}^h \\
-2 \frac{\sigma_{22,1/2,0}}{h_y} - 2 \frac{\sigma_{12,0,1/2}}{h_y} - t_{y00}^h
\end{pmatrix}.
\]

Finally, as an approximation of the equation of state, we choose

\[
[w^h]_{i,j}^{1/2,1/2} = K[q^h]_{i,j}^{1/2,1/2}, \quad \text{where} \quad K = \begin{bmatrix}
\lambda + \mu & \lambda & 0 \\
\lambda & \lambda + \mu & 0 \\
0 & 0 & \mu
\end{bmatrix}.
\]

As a result, a discrete model of the problem is constructed. It has the same structure as the original conjugate-operator:

\[
R_h^* \sigma^h = f^h,
\]

\[
\varepsilon^h = K \varepsilon^h,
\]

\[
u^h = R_h^* u^h.
\]

From it, just as at the differential level, we obtain an approximation of the Lame equations:

\[
R_h^* KR_h u^h = f^h.
\]

In the case under consideration, it is not difficult to show that the constructed difference scheme approximates the original second-order problem on smooth solutions. Its stability can be established by the method described in [7].

We will solve the resulting problem by the method of minimal residuals (the index \( h \) is omitted)

\[
\frac{u^{n+1} - u^n}{\tau_{n+1}} + R_h^* KR_h u^h = f^h,
\]

where \( \tau_{n+1} \) is the iterative parameter, \( n \) – is the iteration number.

4. Simulation results

The constructed difference scheme was tested on a static problem with a solution

\[
u(x, y) = \begin{bmatrix}
\sin(k_1 x) \sin(l_1 y) \\
\sin(k_2 x) \sin(l_2 y)
\end{bmatrix},
\]

where \( k_1, k_2, l_1, l_2 \) – are parameters. The computational domain is \( \Omega = [-\pi, \pi] \times [0, 2\pi] \). At the three boundaries of the domain, stress tensors were specified as boundary conditions. The fourth boundary (right side of the rectangle) was fixed by the condition \( u = 0 \). The vector of mass forces was also calculated using the exact solution.

The calculation results are presented on Fig. 2, 3. The test was performed for \( k_1 = 3, k_2 = 2, l_1 = 2, l_2 = 1, N_x = 100, N_y = 200 \).
Figure 2. Component $u_x$ of the displacement vector

Figure 3. Component $u_y$ of the displacement vector

The obtained test results approximate the exact solution well.

5. Conclusion
A discrete model is constructed for calculating the Lame equation with complex boundary conditions. The model is tested on an analytical solution. A complex boundary condition arises when a microcrack is specified on one of the boundaries. Calculation of microcracks will enable better assessment of the relevance of the simulation and finding out which mechanisms will occur in the case of plasma flow heating in modern plasma and future thermonuclear installations.

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7. References
[1] Vyacheslavov L, Arakcheev A, Burdakov A, Kandaurov I, Kasatov A, Kurkuchekov V, Meikler K, Popov V, Shoshin A, Skvorodin D, Trunev Y, Vasilyev A 2016 Novel electron beam based test facility for observation of dynamics of tungsten erosion under intense ELM-like heat loads American Institute of Physics CP1771, 060004.

[2] Arakcheev A S, Apushkinskaya D E, Kandaurov I V, Kasatov A A, Kurkuchekov V V, Lazareva G G, Maksimova A G, Popov V A, Snytnikov A V, Trunev Yu A, Vasilyev A A, Vyacheslavov L N 2018 Two-dimensional numerical simulation of tungsten melting under pulsed electron beam Fusion Engineering and Design 132, pp. 13-17 [3] Nakamura S, Senoh M, Nagahama S, Iwase N, Yamada T, Matsushita T, Kiyoku H and Sugimoto Y 1996 Japan. J. Appl. Phys. 35 L74

[3] Arakcheev A S, Arakcheev S A, Kandaurov I V, Kasatov A A, Kurkuchekov V V, Lazareva G G, Maksimova A G, Mashukov V I, Popov V A, Trunev Yu A, Vasilyev A A, Vyacheslavov L N 2019 On the mechanism of surface-parallel cracks formation under pulsed heat loads Nuclear Materials and Energy 20 100677

[4] Landau L D, Lifshitz E M 1986 Course of Theoretical Physics VII, Theory of elasticity 196 p.

[5] Konovalov A N, Sorokin S B 1986 Structure of equation of elasticity theory 26 p. [in Russian]

[6] Konovalov A N 1995 Numerical methods in static problems of the theory of elasticity Siberian Mathematical Journal XXXVI, No. 3, pp. 573–589. [in Russian]
[7] Sorokin S B 2015 Justification of a Discrete Analog of the Conjugate-Operator Model of the Heat Conduction Problem *Journal of Applied and Industrial Mathematics*, 9, No. 1, pp. 119–131

[8] Samarsky AA, Andreev VB 1976 *Difference methods for elliptic equations* 354 p. [in Russian]