Application of vectorized algorithms for solving problems of continuum mechanics

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Abstract. The paper discusses the possibilities of constructing vectorized algorithms for solving problems of continuum mechanics, as well as the specialties of their software implementation in the MATLAB. These algorithms, on the one hand, widely use MATLAB functions designed to treat vectors and sparse matrixes, and on the other hand, are distinguished by high efficiency and counting speed.

1. Introduction
Modern computational modeling systems are represented by rather complicated software complexes, designed in the form of application software packages. Today, research and modeling of multiphysical processes in technological systems is inseparable linked with the use of such technologies. However, recently, the issues of creating models, algorithms for performing multivariable analysis of various situations at the research stages, predictive solutions, in which the speed of obtaining the result plays an important role, have become very relevant. Large opportunities within this area are implemented in the MATLAB and related programs in which vectorization operations are supported. Application of MATLAB opens up new possibilities for realization and implementation of finite-difference and finite-volume methods of numerical solution of boundary-value problem in fluid and gas mechanics.

2. Vectorized grid structures
The difference grid covering the calculated area has a structure similar to the structure of a two-dimensional array, which allows addressing to its cells or nodes through a system of two indexes \( i \) and \( j \). A grid node with indexes \( (i, j) \) has neighbors to which it is easy to address, giving corresponding increments of indexes. This addressing principle works both to indicate grid nodes in the finite-difference method and to indicate cells in the control volume method, and such addressing is possible in both physical and computational space.

During programming computational tasks, work with grid structures is usually carried out using a bulkhead algorithm implemented on the basis of nested cycles. This approach involves calculating an index expression and writing the results of the calculations into a two-dimensional array.

Vectorization lets us to work with a lot of data as a single computational structure, which not only makes it compact to write a computational algorithm, avoiding nested cycles, but also increases the efficiency of calculations. You can organize the vectorization of calculations using the tools of modern object-oriented coding languages, in particular, using the MATLAB.
2.1 Addressing internal cells

Consider the principles of constructing vectorized algorithms to solve two-dimensional problems on structured grids. Vectorization in such tasks, excluding nested cycles, is ensured by the appropriate organization of data and the use of vectorized operations.

In fluid and gas mechanics problems, two-dimensional data structures correspond to the fields of hydrodynamic values and the coordinates of grid nodes when solving a problem in a rectangular or curved region, which can be displayed on a computational rectangle using coordinate conversion.

Consider addressing internal cells using the example of an L-shaped calculation grid (figure 1), where for descriptive reasons, a small number of nodes are accepted. The difference grid covering the calculated area has a structure similar to the structure of a two-dimensional array, the addressing to the data in the nodes will consist of specifying two indexes that define the column and the row.

![Figure 1. Addressing internal cells.](image)

In this case, you can use a one-dimensional array to indicate a specific set of nodes of the simulation area. Denote \( C \) the vector of indexes of all internal nodes. In the course of organization a computational algorithm, there is a need for a finite-difference representation of differential operators that appear in equations or boundary conditions. In this case, it is necessary to provide addressing to the data in the neighboring nodes included in the computational template. Using the central cell vector, it is easy to find a subset of nodes that lie to the left of the central cells - \( L \), to the right - \( R \), below - \( D \), above - \( U \), above the left - \( UL \), above the right - \( UR \), below the left - \( DL \) and below the right - \( DR \) (figure 1). The corresponding cell numbers are defined by the following formulas:

\[
\begin{align*}
L &= C - N, & R &= C + N, & D &= C - 1, & U &= C + 1, \\
UL &= C + 1 - N, & UR &= C + 1 + N, & DL &= C - 1 - N, & DR &= C + 1 + N,
\end{align*}
\]

where \( N \) is the number of nodes in the calculation area column.

In computational algorithms implemented using the finite-difference method on a spaced grid or using the control volume method, dummy boundary cells are usually allocated, forming together with internal cells an extended calculation area. The method of addressing dummy boundary cells introduced for setting boundary conditions is explained in figure 2. For this purpose the index vectors \( BL, BU, BR, BD \) are formed and for the considered case there are also \( BRU \) and \( BUR \) corresponding to the left, lower,
upper and right faces of the calculation area. The method of forming these vectors is the same as index vectors of internal cells (angular cells are not used).

Using index representations of grid structures, you can write the difference scheme of the equations by means of one vectorized operator. There is no need to use cycles. This operation of traditional difference schemes replaces the filling of the matrix of coefficients of difference equations, in which each row represents a grid equation and has a high dimension, but it is significantly sparse. Reversing this matrix provides a solution to the problem on the next time layer.

3. Examples of application of vectorized algorithms

The process of convection is determined by the basic laws of conservation of mass, momentum and energy. The peculiarities of the convection problem are exerted in the specificity of forces and flows included in the main equations of the system, as well as in the peculiarities of setting boundary conditions. Generally, for a single-component medium, free convection is described by a system of viscous fluid equations.

3.1 Task of free convection with internal heat source

Using the assumptions of the Bussinesque's model about free convection, the system of equations for solving the problem of free convective flow in variables of the current function - the velocity vortex has the form:

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = -\omega,$$

$$\frac{\partial \omega}{\partial t} + \frac{\partial \psi}{\partial y} \frac{\partial \omega}{\partial x} - \frac{\partial \psi}{\partial x} \frac{\partial \omega}{\partial y} = \nu \left( \frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2} \right) - \beta g \frac{\partial^2 T}{\partial x^2},$$

$$\frac{\partial T}{\partial t} + \frac{\partial \psi}{\partial y} \frac{\partial T}{\partial x} - \frac{\partial \psi}{\partial x} \frac{\partial T}{\partial y} = a \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + \frac{q}{\rho c},$$

where $\frac{\partial \psi}{\partial x} = -v$, $\frac{\partial \psi}{\partial y} = u$ – speed projections to axes of coordinates; $\omega = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}$ – vortex speed; $\rho$ – density; $\nu$ – viscosity; $\beta$ – coefficient of volume expansion; $g$ – acceleration of gravity; $T$ – temperature; $a$ – thermal diffusivity; $q$ – internal source of heat; $c$ – thermal capacity.

System (1) is written for the case of incompressible fluid ($\rho = \text{const}$), which is a consequence of Bussinesque's assumption that the change in density is only taken into account in the expression for gravitational force. A peculiarity of the system is the presence of an internal heat source, whose influence determines not only the parameters of the convective flow, but also the change in the physical characteristics of the medium (viscosity versus temperature).

As an example, we compose a difference scheme for the equation of the current function:
\[
\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \omega = 0.
\]

The difference representation of the second derivative is written as follows:
\[
\frac{\partial^2 \psi}{\partial x^2} = \frac{\psi_L - 2\psi_C + \psi_R}{h_x^2}, \quad \frac{\partial^2 \psi}{\partial y^2} = \frac{\psi_U - 2\psi_C + \psi_D}{h_y^2}.
\]

Then the equation for the current function is written as:
\[
\psi_L + \psi_R + \frac{h_x^2}{h_y^2} (\psi_U + \psi_D) - 2 \left(1 + \frac{h_x^2}{h_y^2}\right) \psi_C - \omega_C = 0.
\]

The problem is solved by the finite-differences method, using the abilities of constructing vectorized algorithms and working with sparse matrices in the MATLAB.

Figure 3 shows the results of simulating free convection with an internal heat source. Figure 3a shows the structure of a 20 x 20 coefficient matrix having 325 zero elements. Figure 3b shows the temperature field.

3.2 Task of free convection with internal heat source

A two-dimensional static problem of the theory of tenacity is considered: the determination of stresses in a flat plate with a longitudinal section. The plate is subjected to external loads applied to two opposite sides so that the normal stress component across the plate is zero. In this case, the plate is in a flat stress state. The solution to the flat stress problem is to determine the stresses \( \sigma_x, \sigma_y \) and \( \tau_{xy} \), which must meet the equilibrium, boundary and compatibility conditions for stresses.

The flat stress problem can be reduced to solving the bigarmonic equation for the Erie function:
\[
\frac{\partial^4 \varphi}{\partial x^4} + 2 \frac{\partial^4 \varphi}{\partial x^2 \partial y^2} + \frac{\partial^4 \varphi}{\partial y^4} = 0. \tag{2}
\]

Equation (2) allows to determine the distribution of stresses in a solid. To solve it, we will use the numerical solution using the finite-differences method. In this case, the area of continuous change of arguments is replaced by a finite set of points - a grid. And the derivatives included in the equation are approximated using the corresponding difference relations.

We make up a difference pattern for strictly internal grid nodes lying in the area bounded by a dashed line. Let’s select any point inside the selected area and take it as the central one (figure 4).
Let's write in the form of finite differences the derivatives included in (2), using the symbols for the nodes shown in figure 4:

\[
\frac{\partial^4 \varphi}{\partial x^4} = \frac{\varphi_{RR} - 4\varphi_R + 6\varphi_C - 4\varphi_L + \varphi_{LL}}{h_x^4}, \quad \frac{\partial^4 \varphi}{\partial x^4} = \frac{\varphi_{DD} - 4\varphi_D + 6\varphi_C - 4\varphi_U + \varphi_{UU}}{h_y^4}.
\]

Figure 4. Differential pattern.

Consider the mixed derivative:

\[
\frac{\partial^4 \varphi}{\partial x^2 \partial y^2} = \frac{\varphi_{UL} - 2\varphi_U + \varphi_{UR} - 2\varphi_R + 4\varphi_C - 2\varphi_L + \varphi_{DL} - 2\varphi_D + \varphi_{DR}}{h_x^2 h_y^2}.
\]

Further, the obtained differential representations of derivatives are substituted in (2).

If you write a difference approximation for each point, then the differential equation is replaced by a system of algebraic equations. Such a system can be written in the form:

\[
A \cdot U = B,
\]

where is \( A \) - a matrix of coefficients of a linear system of equations, \( U \) - is a column vector of unknowns, \( B \) - is a column vector of right parts. To find the vector of unknowns, multiply (3) on the right by the inverse matrix \( A \), then we get:

\[
U = A^{-1} \cdot B.
\]

The following values were used as input: plate size 1 x 1 m; the central incision with a length of 0.2 m. The plate was loaded constant along the length of the edges of the plate with stress, and a quadratic stress distribution law was also set. Quadratic distribution was used in solving a problem without a central section to check the health of the received program.

Figure 5a shows the stress distribution at the edges of the plate, which was set when solving the problem with a plate without a central section. The image is symmetric about the ordinate axis, so half of the graph is shown. As a result of the calculation, the following distribution of normal stresses in the plate was obtained (figure 5b).
This method can be applied to the known problem of loading a cut plate. The accounting of the section and the determination of stresses at angular points is conveniently implemented using vectorized algorithms. Figure 6 shows the result of the solution, where the maximum of normal stresses falls on the angular points of the section. In this case, a constant load is applied to the plate.

**Figure 5.** Stress distribution at the edges of plate (a) and normal stress isolines (b).

3.3 Plate thermal status task

The problem of estimating the unsteady thermal state of an L-shaped plate with local heating is considered. Some of the energy that enters a certain area of the plate is transferred by heat transfer to adjacent cells, and another portion can be radiated from the rear wall of the area. The mathematical model is reduced to the equation of two-dimensional non-stationary thermal conductivity with the addition of two source terms to the right part: the first of them is an energy supply, the second is the loss of heat by the system due to radiation:

\[
\frac{\partial T}{\partial t} = a \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + \frac{q}{\rho c \delta} - \frac{\sigma \varepsilon}{\rho c \delta} T^4, \tag{4}
\]

where \( \delta \) – the thickness of the plate; \( \sigma \) – is the Stefan-Boltzmann constant; \( \varepsilon \) – is the degree of blackness of the plate.

In the vectorized method, a set of all central nodes of the grid, a set of left, right, lower and upper nodes are established (figure 1), as well as a set of boundary nodes (figure 2).

Implicit scheme is used for time sampling (4):
\[ \frac{T_{C}^{n+1} - T_{C}^{n}}{\tau} = a \left( \frac{T_{U}^{n+1} - 2T_{C}^{n+1} + T_{R}^{n+1}}{h_{x}^{2}} \right) + a \left( \frac{T_{D}^{n+1} - 2T_{C}^{n+1} + T_{B}^{n+1}}{h_{y}^{2}} \right) + \frac{q}{\rho c \delta} \frac{\sigma \varepsilon}{\rho c \delta} (T^{n+1})^{4}. \]

In equation (4), the assumption of the constancy of the thermal conductivity coefficient is introduced, but often in non-stationary systems under conditions of intense heating, the dependence of the thermal conductivity on temperature cannot be neglected. In this case, a nonlinearity factor is added. The difference scheme will be recorded as follows:

\[ \frac{(\rho c)_{C} T_{C}^{n+1} - T_{C}^{n}}{\tau} = \left[ \frac{\lambda_{U} + \lambda_{C} T_{U}^{n+1} - T_{C}^{n+1}}{2 h_{x}^{2}} - \frac{\lambda_{C} + \lambda_{L} T_{C}^{n+1} - T_{L}^{n+1}}{2 h_{x}^{2}} \right] + \left[ \frac{\lambda_{U} + \lambda_{C} T_{U}^{n+1} - T_{C}^{n+1}}{2 h_{y}^{2}} - \frac{\lambda_{C} + \lambda_{D} T_{C}^{n+1} - T_{D}^{n+1}}{2 h_{y}^{2}} \right] + \frac{q}{\delta} \frac{\sigma \varepsilon}{\delta} (T^{n+1})^{4}. \]

In the implicit difference scheme, radiation is included by a term of the right part having a fourth order temperature factor. Implicit inclusion of this term introduces another factor of significant nonlinearity. Let’s linearize this term according to Newton, then the difference representation of this ratio can be written in the following form:

\[ (T^{n+1})^{4} = (T^{n})^{4} + \frac{\partial T^{4}}{\partial t} \tau = (T^{n})^{4} + \frac{\partial T^{4}}{\partial T} \frac{\partial T}{\partial t} \tau = (T^{n})^{4} + 4(T^{n})^{3}(T^{n+1} - T^{n}) = 4(T^{n})^{3}T^{n+1} - 3(T^{n})^{4}. \]

Figure 7 shows the result of the system solution (4).

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4. Conclusion

An approach to the form and implementation of vectorized algorithms for solving problems of continuum mechanics has been developed. As specific examples, the problem of free convection with an internal heat source, the problem of the concentration of stresses in the cracks of the structure, the problem of the thermal state of the plate are considered.

Developed algorithms are used to solve more complex problems of continuum mechanics. Among these problems are construction tasks for areas of complex geometric configuration, which requires the construction of curved grids; tasks of calculation of currents in inflatable channels and a number of other problems. Vectorization allows you to consider the motion of the complex of the vectorized set of particles in the continuum mechanics, as well as vectorization allows you to conveniently model vortex structures. Created software tools can be used to support scientific research in various fields where mathematical modeling methods are used.
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