Effective Use of Sparse Matrices in Problems of Mathematical Modeling

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Abstract

Mathematical modeling and the related computer experiment are now one of the main means of studying objects, processes and phenomena of various nature: in science, engineering, economics, society, etc. A significant improvement in the quality of mathematical modeling in many areas of science and engineering is possible only with the use of fundamentally new three-dimensional models, the transition from computer simulation of individual components and assemblies to the calculation and optimization of the product as a whole. It is obvious that the consideration of problems in such a formulation leads to discrete mathematical models of super-large sizes. Existing supercomputers of different parallel architectures make it possible to efficiently solve such problems. However, the time for solving problems on parallel computers consists of the time of the actual solution and the time of performing additional operations, that are necessary for the exchange of information between computing devices, that is overhead costs. This is especially true for problems of linear algebra with different structures of sparse matrices of large volumes, that arise in the mathematical modeling of processes. Sparse matrix compaction schemes, decomposition of data arrays between processors are one of the main factors for the effective solution of these problems on parallel computers. The paper considers efficient methods for processing sparse matrices of arbitrary structure for the purpose of effective mathematical modeling of structural strength problems on parallel computers. Various methods of regularization and decomposition of sparse matrices of arbitrary structure, efficient data storage schemes, technology for studying the conditionality of a matrix with approximate data on a computer are proposed. This way of using sparse matrices in mathematical modeling ensures more efficient use of computing resources and reliability of computer results. Problems of mathematical modeling are presented, where the considered methods of processing sparse matrices were effectively applied.

Keywords

Mathematical modeling, structural strength problems, sparse matrices, linear algebra algorithms, methods of structuring sparse matrices

1. Introduction

Nowadays, one of the main directions of scientific and technical progress is the mathematical modeling of complex objects, processes, and phenomena, which is the basis of modern applied developments in various fields of science and technology. With the advent and constant development of supercomputers of various architectures, the problems of their effective use, the expansion of the range of tasks that need to be solved, and the assurance of the reliability of computer results become very relevant. As a practice and literary sources show, mathematical modeling of 80-85% of all

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scientific and technical problems is reduced to solving problems of linear algebra - systems of linear algebraic equations (SLAE) and algebraic eigenvalue problem (AEVP) for sparse matrices of various structures. The efficiency of solving the entire problem of mathematical modeling largely depends on the efficiency of solving these problems.

Despite the fact that there is a huge amount of software for solving linear algebra problems on various computer architectures on the international market, new applied problems are appearing that require new efficient algorithms. This is primarily due to the difference in the types of matrices (dense and sparse), structural properties (band, arbitrary structure, triangular and others), mathematical properties (singular and non-singular, positive definite, sign-definite etc.), and ways of processing them on different computer architectures.

2. Mathematical modeling of problems streng structurals and stability of new composite materials

When designing objects for various purposes, it often becomes necessary to carry out calculations of the strength of structures of the whole objects and their individual elements. Such problems arise, in particular, in various branches of mechanical engineering (ship building, aircraft building, rocket building, engine building, etc.), in industrial and civil engineering (calculation of individual structural elements or structures as a whole), etc.

Increasing requirements for the quality of design solutions, the use of new constructive materials lead to the development of refined three-dimensional mathematical models with huge amounts of processed information. Despite the availability of powerful supercomputers of different architectures, there is a need to use efficient methods of computer data processing, the volume of which is constantly growing.

2.1. Mathematical formulations of structural strength problems

Mathematical problems of calculating the strength of structures using the principle of possible displacements are reduced to the following variational problems [1]:

It is necessary to find a vector function that $u \in U_0$, for any possible displacement $v \in U_0$ satisfies the integral identity

- for a static problem

$$a(u,v)=l(f,v); \tag{1}$$

- for dynamic problem

$$a(u,v)+b¿ \tag{2}$$

$$u(t_0)=u^{(0)}, \quad u(\{t\} \text{ rsub } \{0\})= \{u\} \wedge \{(1)\} \tag{3}$$

- for the problem of eigen oscillations

$$a(u,v)=\lambda b(u,v) \; ; \tag{4}$$

where U_0 – is the infinite-dimensional functional space of possible displacements; symmetrical bilinear forms $a(u,v)$, $b¿$, $c(u',v)$ symmetrical bilinear forms are proportional in accordance with the potential, kinetic energy of deformation and braking energy, and the linear form $l(f,v)$ is proportional to the work of the applied (external) forces under load. The first time derivative of the vector function $u(t,\chi)$ is denoted u', and the second u .

Only linear problems are considered here, since it is assumed that the solution of a nonlinear problem can be reduced to solving a sequence of linear problems.

2.2. Discretization of problems of mathematical modeling of structural strength

The theoretical basis of most software tools for calculating the strength of structures, for example, the SP LIRA software package designed to solve problems of calculating the strength of building structures [2–4], is the finite element method (FEM) [5], implemented in the form of displacements. The choice of this form is explained by the simplicity of its algorithmization and physical interpretation, the availability of unified methods for constructing stiffness matrices and load vectors for various types of finite elements, the possibility of taking into account arbitrary boundary conditions and the complex geometry of the estimated structure.

To obtain a discrete problem with the help of the FEM, the area occupied by the structure is distributed into finite elements, nodes and their degrees of freedom (displacement and rotation angles of nodes) are assigned. The degrees of freedom correspond to the basic (coordinate, approximating) vector-functions ϕ_i, of nonzeros only on elements containing a node corresponding to a given degree of freedom. In addition, the following relations hold for the degrees of freedom and basis functions

$$L_j(\phi_i)=\delta_{ij}, \tag{5}$$

where δ_{ij} – is the Kronecker symbol, and the result of the operation $L_j(\phi_i)$ is the value of the component component of the vector-function ϕ_i for the degrees of freedom L_j.

Approximate solutions of the corresponding problems are sought in the finite-dimensional subspace U_0^h of space U_0. Vector-functions from subspace U_0^h are piecewise polynomial and can be represented as a linear combination of basis vector-functions, which satisfies the main (kinetic) conditions for a linear combination of basis vector-functions

$$u_h(\chi)=\sum_{i=1}^{n} x_i \phi_i(\chi), \tag{6}$$

where $\phi_i\ (i=1,2,\dots,n)$ – the piecewise polynomial basis mentioned above U_0^h.

Then the discrete problems, that should be solved have the form [6]:

- systems linear algebraic equations for a statistical problem (1)

$$Ax=b; \tag{7}$$

- problems with initial conditions for dynamic problem (2), (3)

$$Bx''(t)+Cx'(t)+Ax(t)=b(t),\ \ x(t_0)=x^{(0)},\ \ x'(t_0)=x^{(1)}; \tag{8}$$

- algebraic eigenvalue problem for the problem of eigen oscillations (4)

$$Ax=\lambda^h Bx. \tag{9}$$

2.3. Mathematical formulations of structural (composite materials) stability problems

To investigate the sustainability of composite materials, the static method of the three-dimensional linearized theory of stability is used within the framework of the second version of the theory of small subcritical deformations. The subcritical state is determined from the solution of the plane problem of the linear theory of elasticity of piecewise homogeneous bodies for various boundary conditions, which correspond to a three-layer element of periodicity in the case of a material and a three-layer element of a structure with lateral sides free from stresses in the case of a composite sample [7].

When using the static Euler method, the stability problem is reduced to a generalized eigenvalue problem of the form (9), in which the minimum (in general, modulo) eigenvalue determines the critical load, and the corresponding function determines $u_k(u_{k,1},u_{k,2})$ – the form of stability loss. The following are accepted as the main mathematical models: the equation of the linear theory of elasticity of piecewise homogeneous environment to determine the subcritical stress-strain state; equation of the three-dimensional linearized theory of stability at small deformations to determine the critical parameters. The model of a piecewise homogeneous medium is used as a mechanical model. Composite components are modeled by linearly elastic isotropic bodies [7].

Thus, for a plane deformation, we obtain an eigenvalue problem for a system of partial differential equations with variable coefficients depending on two variables. In this case (the investigation of the stability of a composite material under a compressive load), the conditions of selfadjointness of the operators of the problem of determining the initial stress-strain state and the generalized eigenvalue problem are satisfied, which corresponds to the problem of three-dimensional stability theory. In addition, the differential operators of the problems under consideration are positive-definite under the condition that there is no rigid displacement.

2.4. Discretization of problems of mathematical modeling of structural (composite materials) stability

For the numerical solution of the problem of the three-dimensional linearized theory of stability and the problem of the linear theory of elasticity, a discrete model is used, which is constructed by the variational-difference method (finite differences) using the concept of basic schemes. In the computational domain, with the help of straight lines, a difference grid nonuniform in each direction is introduced so that the material is homogeneous within one grid cell. Thus, the discrete problem of determining the subcritical stress-strain state (the problem of the linear theory of elasticity) is written in the form of an SLAE of the form (7) with a sparse symmetric positive definite matrix. The discrete problem for the stability problem is written in the form of a generalized AEVP of the form (9) of sparse symmetric positive definite matrices [7].

2.5. Increasing the efficiency of mathematical modeling on a computer

In order to provide an effective computer solution of problems (7)–(9), it is necessary to take into account the following features [4, 7, 8]:

- matrices of discrete problems – stiffness A, mass B, damping C are symmetrical, positive definite or positive semidefinite, and have a sparse structure (band, profile, block, etc.; a matrix is called sparse if the number of its non-zero elements is much less than their total number n^2, where n is the order of the matrix) [1, 6].
- the order of the matrices of the discrete problems to be solved is $O(10^5)-O(10^8)$, in the near future the era of exascale computing is coming [8, 9];
- elements of matrices and vectors that occur in the process of mathematical modeling are calculated with errors caused by errors in the original data, discretization errors, and errors in calculating the values of these data on the computer [8].

Therefore, for the effective use of computing resources of modern supercomputers in the mathematical modeling of structural strength problems with approximate data and ensuring the reliability of the obtained computer results, it is necessary:

- identify the original structure of the sparse matrix;
- determine the need for structural regularization and choose the most efficient (for a given computer architecture) regular structure of matrix;
- carry out structural regularization of sparse matrices - reducing an arbitrary initial structure of matrix to a regular block-sparse one (block-tape, block-profile, block-skyscraper, block-diagonal with bordering, etc.);
- choose or develop the most efficient (for a given computer architecture, taking into account the regularized structure of matrices) parallel algorithm for solving the problem;
- choose, in accordance with the algorithm, a decomposition of matrices scheme (the distribution between processor devices of a parallel computer);
- choose, in accordance with the algorithm, the scheme for storage of matrix elements in a computer;
- investigate of the correspondence the mathematical properties of the matrix, entered into the computer, with approximate data and the functional purpose of the algorithm for solving the problem.

Such a scheme for researching and solving SLAE and AEVP for sparse matrices of various structures is implemented in the created parallel algorithms for modern computers with parallel organization of computing, namely for MIMD-architecture computers with multi-core processors and hybrid architecture [4, 7, 8].

3. Ways for structural regularization, decomposition and storage of sparse matrices for efficient modeling of structural strength

The structure of non-zero elements (the structure of a sparse matrix) is determined by the numbering of unknown problems and can be either regular (for example, band, profile, block-diagonal with framing, etc.), or irregular (arbitrary). The structures of factorization matrices can be obtained by performing the so-called symbol factorization of the initial matrix. In most software tools, before forming the matrices of calculation problems, the unknowns are renumbered (i.e., the sparse structure is reorganized) in order to reduce the total number of floating-point arithmetic operations when solving calculation problems. Figure 1 shows the structures of matrices (actually factorized matrices) of calculation problems that arise when modeling the stress-strain state of structures.

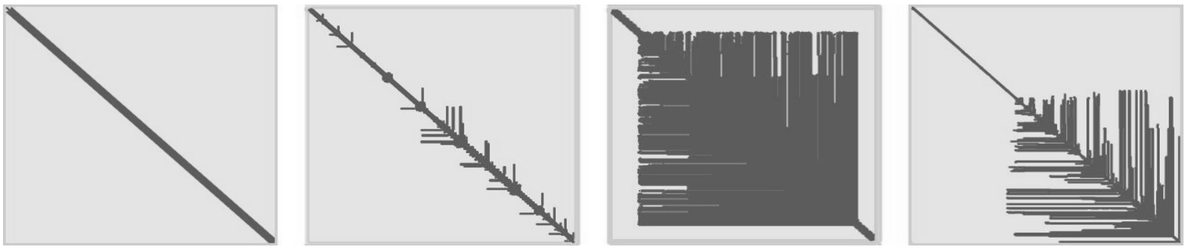

Figure 1: Examples of Sparse Matrix Structures

3.1. Reduction of sparse matrices of arbitrary structure to a regular form

Problems of solving linear algebra problems with sparse matrices and ways to solve them are considered in [10–13]. There are a number of methods that allows to control the filling of the matrix when solving problems on computers. Both methods of general purpose [10, 11] and those oriented to matrices of a specific type [12, 13] have been developed. Depending on the task and features of the matrix, it is possible to optimize its portrait by changing the width of the tape, reducing the profile of the matrix, adjusting the total amount of filling, and bringing the structure to a certain form [10, 11].

Among these methods, the following should be mentioned:

- • the Cuthill-McKee method and the factor tree method – the use of these methods ensures the concentration of non-zero elements as close as possible to the main diagonal, which, as a rule, makes it possible to represent the matrix in a band or in profile form;
- • method of parallel sections – the use of this method makes it possible to represent the matrix as a block-diagonal (with large diagonal blocks) with a border (the order of the diagonal frame block should be much less than the orders of the main diagonal of blocks) [10, 11];
- • minimum degree method – when using this method, as a rule, a reordered matrix is obtained, for the development of which fewer arithmetic operations are required; the resulting structure is called "skyscraper" [2–4] because this structure resembles the skyscrapers of Manhattan (figure 2).

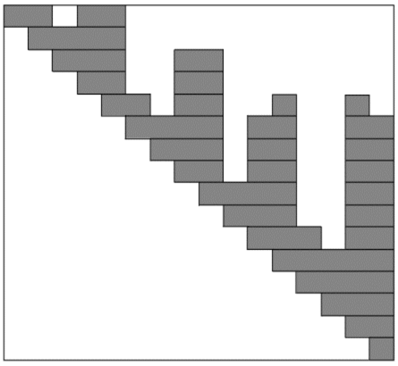

Figure 2: Portrait of the upper triangle of the "skyscraper" matrix

Discrete problems with matrices of this type arise in the problems of calculating the stability of structures. For effective implementation in algorithms, for example, matrix-matrix operations of sparse matrices, it is advisable to first reorder (or immediately form) them so that the vast majority of nonzero elements are located in the most dense matrix blocks: i.e, determine zero blocks (all elements are identically equal to 0) and non-zero (have at least one non-zero element). It is also desirable that non-zero blocks are filled as much as possible. The block sizes are determined based on the architecture of the computer.

If in the future it is supposed to use the decomposition of the sparse matrix into the product of triangular matrices (e.g., LU, LL^T, etc.), then it is necessary to determine the block-sparse structure of the decomposition matrices using the symbolic decomposition of the original matrix. After that, it is necessary to optimize the block-sparse structure of the original matrix or decomposition matrices, using one of the above algorithms and replacing the matrix elements in the algorithms with blocks. In many cases, it is expedient to combine adjacent (in a row or column) non-zero off-diagonal blocks of the optimized matrix structure into one rectangular block (tile), which will be further processed as a whole. In some cases, it is advisable to optimize the structure of diagonal blocks to reduce the number of arithmetic operations with individual blocks of the resulting block-sparse matrix.

Consider another type of sparse matrix – a bordered block-diagonal matrix (figure 3).

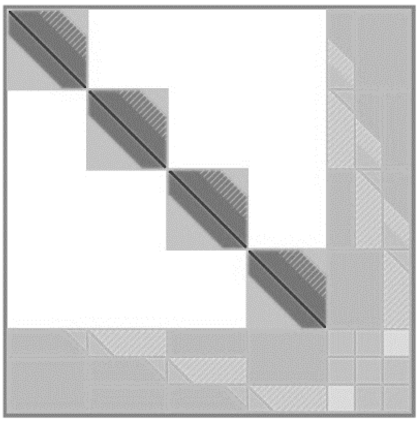

Figure 3: Block-Diagonal Bordered Matrix (p = 4)

Discrete problems with matrices of this type appear, for example, when solving boundary value problems by the finite element method or the finite difference method, if the domain is divided into subregions and discretization is carried out, and the unknowns of the discrete problem are numbered in the following order. First, the unknowns that belong to only one subregions, sequentially through the subregions. Then, in the same order, the unknowns belonging to two subregions, then three, and so on - these unknowns form a border. For efficient parallelization, it is necessary that the dimensions of the diagonal blocks corresponding to the unknowns of one subregions exceed the dimensions of the border of the diagonal block by an order of magnitude or more.

3.2. Decomposition (distribution schemes) of sparse matrices

Many methods for solving linear algebra problems, that is used in modeling structural strength problems, are based on algorithms for decomposing a matrix into a product of matrices of standard types, for example, lower and upper triangular matrices. Such algorithms are characterized by a gradual decrease from step to step in the size of the processed part of the matrix. Therefore, it is important to ensure approximately the same amount of calculations, exchanges and synchronizations performed by each process or thread on a parallel computing model, that is, to exclude the influence of the Haydn effect [8, 14, 15].

As research has shown, parallel versions of these algorithms, in which the so-called cyclic distribution schemes and processing matrices are created (see, for example, [8, 14, 15]), provide a sufficiently good load balance of processes (flows).

Quite often, one-dimensional block-cyclic schemes are used: rows or columns of non-zero blocks of the matrix are distributed cyclically between processes or threads of the upper level of parallelism, for example, if the q-th process is distributed elements of matrix rows with numbers $sr+1,\dots,sr+r$, then $(q+1)$ -th process will have rows with numbers i-th process will have rows with numbers $s(r+1)+1,\dots,s(r+1)+s$, where s is the number of rows in the block (we can talk about the r-th and (r + 1)-th rows of square matrix blocks of order s).

In the case of a regular sparse matrix structure, parallel algorithms that use one-dimensional block-cyclic schemes for allocating matrix elements can provide an approximately equal amount of computations and exchanges performed by each parallel process or thread at each instant of time (see, for example, [8, 14, 15]).

Such a regular structure is primarily the band structure of the matrix under the obvious condition that the half-width of the matrix band m exceeds the product $s\times p$, where p is the number of processes or threads. In the case of a regular profile structure of the system matrix, by varying the value of s and p, one can practically balance the load of parallel processes at each moment of time if $c_e/n>sp$, where c_e is the total number of subdiagonal elements in the matrix profile.

For block-diagonal bordered matrices, cyclic distribution schemes do not allow balancing the load of processes, and it is advisable to use block distribution schemes between computational elements. That means that each diagonal block, together with the corresponding off-diagonal border block, is distributed to a separate process (or thread). A diagonal border block can also be allocated in a separate process (or thread).

There are various storage schemes for sparse matrices, that differ in the way zero elements usage. In some cases, it is allowed to store a portion of zeros in exchange for simplifying the storage scheme; in others, all zeros of the matrix are used; thirdly, zeros are not used at all. The choice of storage format, of course, affects memory requests, and therefore significantly affects the efficiency of software implementations of algorithms for processing sparse matrices (for example, decomposition of matrices into a product of triangular matrices).

In the algorithms created for solving SLAE and AEVP, different formats for storing elements of sparse matrices are used: *coordinate* format, *sparse row or column* format, *ELLPACK* format, *hybrid* format, etc. [4, 8].

3.3. Investigation of the mathematical properties of matrices entered into the computer

Mathematical models describing applied problems always contain errors in the initial data [8]. That is, a characteristic feature of mathematical models with approximate data is that their mathematical properties are a priori unknown. Within a given level of error, problems can be both compatible and incompatible, both correctly and incorrectly stated, both poorly and well conditioned. Due to the rounding error, a nonsingular matrix can become degenerate in a computer, and a degenerate matrix can become nonsingular. There is a problem of choosing the necessary algorithm for solving the computer model of the problem with the reliability of the results obtained.

An error in the solution of a mathematical problem, which is caused by an error in the initial data set, is called a hereditary error. If the hereditary error of the solution of a mathematical problem is large, then the obtained mathematical solution may not have a physical meaning, that is, such a solution will not contain the solution of a physical problem. Therefore, it is necessary to determine the scope of the mathematical model, because the hereditary error cannot be corrected by mathematical methods of solving the problem. To reduce the hereditary error, you can either increase the accuracy of the input data or reformulate the problem with respect to other parameters [8].

The investigation of the correctness of the problem statement in a computer is reduced to checking two relations:

$$1.0+\gamma \neq 1.0, \quad (\|\Delta A\| \|A\|) h(A) < 1; \tag{10}$$

where $h(A)$ – is the condition number of the system matrix, $\gamma = h^{-1}(A)$. The first condition, fulfilled in floating-point arithmetic, means that the matrix is non-singular within the limits of machine accuracy (machine non-singular), and the second one means that it is non-singular within the limits of the accuracy of the input data [8, 16].

Thus, when conditions (10) are met, the solution of the computer problem with approximate data exists, is unified and stable. Such a computer task should be considered as correctly posed within the accuracy of the initial data input. Otherwise, the matrix of the system may turn out to be a matrix of incomplete rank, and the computer problem should be considered as incorrectly posed. The fulfillment of condition (10) at an increased computer bit rate in accordance with the value of the condition number of the matrix indicates that the original problem is poorly conditioned relative to the previous bit rate and it is possible to obtain a single solution at an increased bit rate.

So, the computer problem, which should to be solved in the end, always has approximate data relative to the original problem (due to the hereditary error in the initial data, due to the discretization errors, due to the errors in obtaining numerical data in the computer).

In the created parallel algorithms for solving SLAE and AEVP for sparse matrices of various structures on modern high-performance computing systems with parallel organization of calculations, a research is provided in a computer environment of the mathematical properties of matrices using various computer bit rate (the technology is described in the work [16]).

4. Using effective ways of structuring sparse matrices in some practical problems of mathematical modeling of structural strength

Let's consider some practical problems of mathematical modeling of structural strength, which are reduced to solving linear algebra problems with sparse matrices.

To analyze the strength of building structures on single-processor computers, Software package Lira-Sapr is widely used – a multi-threaded version of PC Lira [17]. The developed parallel algorithms for solving SLAE with sparse matrices of various structures were used as a processor component of the parallel version of PC Lira – the software package Lira-cluster [2–4, 18].

Consider the problem of analyzing the strength of a 27-storey building (figure 4). The sparse symmetric matrix obtained as a result of discretization by the finite element method (FEM-mesh) has an order of 661590 and a band half-width of 34242, density (the matrix tape is filled with non-zero elements by 5%). After optimizing the matrix structure by the minimum degree method, a skyscraper structure matrix was obtained (order – 661590, ribbon width – 541257, density <1%). The time for solving the problem using Lira-Sapr on a personal computer is 3254 sec, using Lira-cluster on the hybrid architecture of the SKIT-4 supercomputer is 57 sec. Thus, an acceleration of 23 times was achieved.

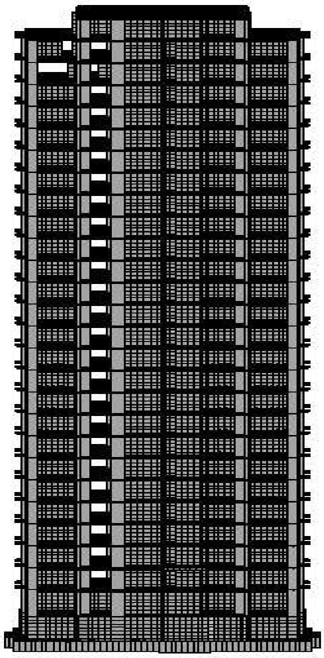

Figure 4: FEM-model of a 27-storey building

Supercomputer SKIT-4 of the V.M. Glushkov Institute of Cybernetics National Academy of Sciences of Ukraine has the following specifications: CPU – Intel(R) Xeon(R) CPU E5-26700, clock speed 2.60 GHz, speed 8 GT/s, cache memory – 20 MB, per node: 2 CPUs with 8 cores + Hyperthrefding =32 cores, Max Memory Size – 384 GB; GPU – Nvidia Tesla M2050, 3 GB memory, peak performance – 515 Gflops [19].

4.1. Numerical investigation of the stability of composite materials

The created parallel algorithms for solving SLAE and AEVP for sparse matrices of various structures were used in mathematical modeling of the problem of structural stability - the problem of stability of a layered two-component composite material with a regular structure (Fig. 5, left) under a uniform single-axis load on computers of various architectures. Since the stability problem is solved for the computational domain of finite dimensions (Fig. 5, right) and the influence of the boundary conditions on the lateral sides of the computational domain on the critical stability parameters is studied, we distinguish between the loss of stability in a composite material and a composite sample corresponding to this material [7, 20, 21].

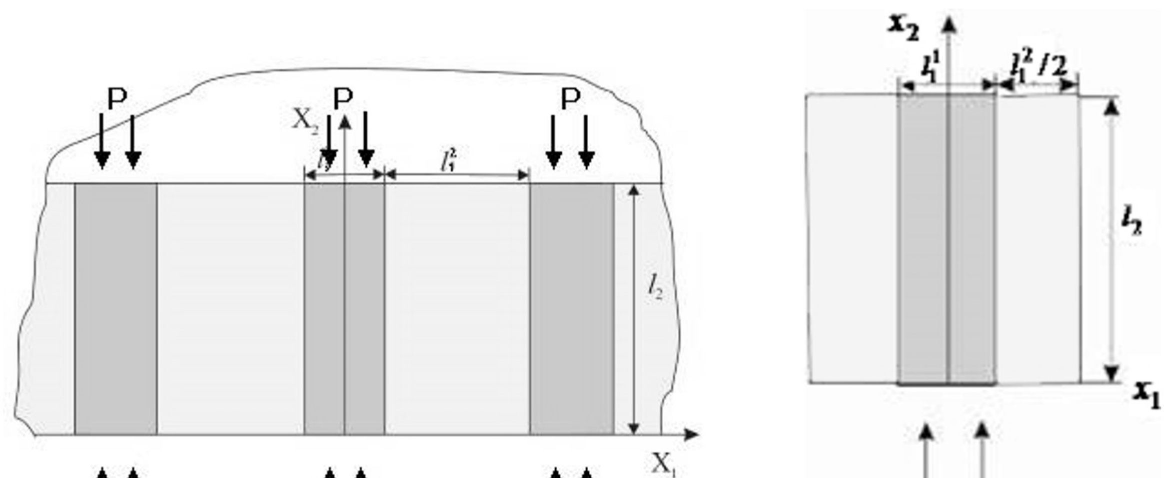

Figure 5: Schematic representation of the stability problem

The problem of mathematical modeling of the stability of composite materials was solved on a parallel computer of hybrid architecture SKIT-4.

Comparative results of solving the obtained partial generalized eigenvalue problem $Ax = \lambda Bx$ in the problem of mathematical modeling of the stability of new composite materials are given for band symmetric positive definite matrices (the order of matrices A and B is 12282, the half-width band of matrix A is 6212, the half-width tape of the matrix B is 71).

Compared to the sequential version of the algorithm, the case of solving the AEVP of band symmetric matrices, a 7-fold acceleration was obtained by the parallel algorithm on the MIMD architecture; on a hybrid architecture - 18 and 33 times, using one and two GPUs respectively compared. In the case of the AEVP solution for sparse matrices reduced to the block-diagonal form with border, an acceleration of 43 times was obtained on the hybrid architecture using two GPUs compared to the sequential version of the algorithm [21].

5. Conclusions

Methods for regularization, decomposition and storage of sparse matrices are proposed, which allow to significantly increase the efficiency of solving problems of mathematical modeling of structural strength. New methods and computer block-cyclic and block algorithms for high-performance computing created on their basis for solving linear algebra problems (systems of linear algebraic equations, algebraic eigenvalue problem) with approximate data can be used for mathematical modeling of different processes on modern supercomputers.

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