Developing the Method and Software for Calculating Layered Medium Flows in Parallel

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The modern development of computing systems can essentially increase efficiency of the solution of scientific and engineering problems. The new outcomes are reached at system development and programs intended for problem solving, limiting in relation to capabilities of computer facilities. In this area parallel computing systems and parallel programming are of the greatest concern.

The calculation of viscous flows with thin layers is one of the most topical computing problems of simulation. The lamellar structure of flow essentially influences processes of carrying mass and impulse across layers, and also the speed of energy dissipation. One of perspective approaches is founded on the potential theory for the description of slow flows and its numerical approximation by the boundary element method (BEM).

The necessity of discretization only the boundaries of investigated structure is one of the advantages of BEM. That results in much lower order of equation systems, than in other methods, and also in efficiency and accuracy of high-gradient fields calculation.

The problem solving in case of small and thin areas is usually connected with computing instability and loss of accuracy, when small changes of input data correspond to an inadequate change of the solution. BEM is not an exception, using this method may result in computing instability, connected with proximity of the boundaries of researched structures thin areas and usage of velocity integral equations. So obtaining the satisfactory numerical solution in these conditions represents one of the important problems of computing simulation. The ordinary way of finding its solution is the use of averaging methods, and classic equations of small-sized water. At the same time there is a detailed theoretical base of regularization methods, but, it is required, however, to construct effective, parallelizable and having sufficient universality numerical algorithms realizing those methods.

Problems of parallel calculations are among of the most actual computing problems: developing and researching parallelizable numerical methods which are well scalable using several computers in a cluster in order to achieve the greatest efficiency of their usage; analyzing algorithms structural properties; constructing and architecture of computational systems; using clusters in calculations.

Taking into account the features of a researched problem and adapting both numerical algorithms and software carrying out calculations and effective information exchange between computing environment participants is very important for rising significance of newly created numerical methods and software. There are many facilities supporting parallelizing (MPI, OpenMP, PVM, languages: C-DVM, FORTRAN-DVM etc.), ensuring portability and message exchange between computational nodes, that, however, requires strong binding to such systems and might not be optimal regarding the speed of calculation owing to not taking in mind particular features of the solving problem. Therefore, the task of developing more specialized software taking into account the features of a problem and having a sufficient universality and flexibility remains actual.

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The statement and solution of the boundary element method generalization problem for calculation of flat and three-dimensional flows of viscous liquid with a free surface on a case of layered structure of flow at small Reynold's numbers are given. The problem is reduced to the solution of an integral equations system with isolated singularity for fictitious forces. The equations of this system meet boundary conditions and continuity conditions of pressure on boundaries of liquids separation.

The boundary-element solution of a considered problem can be found by dividing these boundaries on straight-line sections or triangular elements adjoining to each other and supposing that fictitious forces within the limits of each section are constant.

When considering layered flows integral equations of first kind are used on inner boundaries.

According to the carried calculations it leads to an ill-conditioned linear equations system not having diagonal predominance. The obtained equations are almost indistinguishable for close boundary elements. This circumstance results in impossibility of obtaining of a correct numerical solution by direct using of well-known linear systems solving methods. It is confirmed by outcomes of the special trial of methods applied to the obtained systems such as Seidel method, conjugate gradient method, Gauss method with full sampling and square root method. Iteration methods demonstrated the divergence of discrepancy from the first iterations. Direct approaches produced the solution disharmonious with the physical nature of considered problems. It is discovered that small changes of geometry of investigated bodies or applied loads correspond to the considerable and uncoordinated change of outcomes.

To deal with the detected solution instability the algorithm of obtaining the steady solution, founded on the regularization method by Tikhonov is developed.

This method is formulated as a variational problem of functional minimization:

$$f(x) = \|Ax - b\|^2 + \alpha \|x\|^2, \quad (1)$$

where $\alpha = \alpha > 0$ is a regularization parameter, A is the matrix of a linear equations system, b is a boundary conditions vector.

The solution (1) is regularized, and, therefore, steady. The minimum of the functional (1) is provided by solving the following system:

$$\left(A^* A + \alpha E\right) x = A^* b + \alpha x_0, \quad (2)$$

The approach that can easily be implemented in practice of finding a regularization parameter consists in creating and solving linear equations systems repeatedly by well-known methods. The algorithm includes external and internal cycles providing fulfilment of obtaining a regularized solution.

External cycle creates a reducing to zero sequence $\{\alpha_p\}$, on units which one the minimization of the functional (1) takes place. The geometrical progression $\alpha_{p+1} = \mu\alpha_p$, $p = 0,1,2,\ldots$, $\mu < 1$ can be taken as such sequence. After selecting the next $\alpha = \alpha_p$ the transition to internal cycle follows.

Internal cycle provides searching the minimum of the functional (1) at the fixed value $\alpha = \alpha_p$.

After that the transition to the external cycle follows.

The vector of boundary conditions is used as the vector x_0 at $\alpha = \alpha_0$ and on each subsequent iteration the vector x_0 is a regularized approximation x obtained from previous one.

The number of internal cycles and the stopping criterion depends on a particular problem. The discrepancy criterion using regularized approximation obtained at each iteration of the internal cycle is one of most reliable.

The technique and outcomes of developed algorithms testing are presented.

It is also determined that the time expended for calculations increases in case of using of the regularization technique. Practical problems, depending on the geometry of investigated

bodies, the density of boundary elements and the accuracy of calculations, may lead to increasing of calculation time in geometrical progression.

Such time expenses make topical developing of the algorithms and software of calculating of liquids with layers based on the concept of parallel calculations.

The developed software product "PHS" solving the problem of organizing and carrying out of a parallel calculation is described. The purpose of its creation is the effective organization of collecting of the input data describing a problem being solved and automation computing at all stages of a calculation with load distribution on a cluster of workstations.

The program consists of two large parts. The first solves problems on automating of data input and storage, implementing of body discretization numerical algorithms, constructing and solving of a set of equations using one computer, calculating of flow diagrams and their saving in the GIF format. It is entirely situated on one computer, where all the calculations are carried out and the outcomes are saved.

The second part solves a number of problems on organizing of calculations on a cluster of workstations connected by local network.

The way of the functional (1) minimization is the mathematical basis permitted to carry out calculations in parallel. The immutable parts, namely products A^*A and A^*b, can be calculated only once. In addition the operation of multiplying of the transposed matrix on the matrix itself can be easily carried out by workstations in parallel using the same mathematical algorithm as on supercomputers with distributed memory. The sequential solving of linear equation sets with different $\alpha = \alpha_p$ also can be carried out in parallel. It is possible due to using the square root method to solve such sets. As it is not required to know the previous iteration outcomes of internal cycle calculation during forward trace of this method, these calculations for different $\alpha = \alpha_p$ can be carried out in parallel. After finishing transformations by one of computers of the matrix for $\alpha = \alpha_p$ the outcome has to be sent to the computer calculating iteration for $\alpha = \alpha_{p+1}$, etc. The saving of time occurs due to spending much more time to carry out the forward trace calculation in comparison with the return trace.

The application outcomes of the developed algorithms and programs for solving a problem of filling a flat and prismatic vertical channel with viscid layered liquid are presented.