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The most parallel computing algorithms for solving tasks of heat and mass exchange

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Abstract
Problems of mathematical modeling of Dirichlet problems are considered on the basis of use of parallel computing systems of cluster type. For solution of multivariate spatial tasks, it was offered to convert the task of three-dimensional distribution in the field of variables change to the sequence of the diagrams excluding unknown values only in one direction – alternately in longitudinal, cross and vertical. For this purpose it is recommended to use implicit schemes; it leads to systems of the linear algebraic equations with three-diagonal structure. It is shown that the greatest effect of the parallel processor is reached by application of elements of the linear algebra for matrix computation. In this regard, special attention is paid to development of the maximum parallel forms of algorithms of the differential schemes with three-diagonal structure. It is shown that the offered algorithm of a cyclic reduction of shifts allows the highest level of vectorization. Application of a method of "odd-even" reduction of lines for system of the linear algebraic equations allows to us to develop the parallel algorithm with the maximum extent of vectorization.
Key words: HEAT CONDUCTIVITY EQUATION, METHODS OF PARALLEL CALCULATIONS, PARALLELIZATION ALGORITHMS

Problem statement and analysis of the last achievements in this field

Relevance of a problem of numerical methods development for the solution of multidimensional systems of the parabolic quasilinear equations describing processes of heat and mass exchange is beyond doubt. One of the most interesting examples of such systems can be equations of hydrodynamics and metallurgical thermophysics [1, 2]. By now, there appeared such situation when one-dimensional non-stationary tasks can be solved with an accuracy sufficient for the majority of technical inquiries. At the present level of technical capability and on the basis of the existing traditional methods, apparently, it is possible to speak about the mass solution of three-dimensional non-stationary problems of heat conductivity only considering the following circumstances.

Firstly, emergence of modern and inexpensive means of communication of computer facilities stimulated development of the new information technologies (IT), to which the systems of parallel information processing belong. Organization of parallel processing of information streams, connection of problems of parallelization with architecture of PC, system of parallel programming, methods and algorithms of parallel calculations are those essential phases of development of computer facilities at this stage [3−5]. Secondly, certain tendencies of development of the computing methods with complex logical structure having higher order of accuracy in comparison with traditional final and differential methods were outlined [6 − 8]. As serious progress in area of solving multivariate spatial tasks can be considered a row of the suggestions pursuing one stereotypic aim – to convert the task of three-dimensional distribution of area of variables change to the sequence of the diagrams excluding unknown values only in one direction – alternately in longitudinal, cross and vertical. Use of implicit schemes leads to the systems of the linear algebraic equations (SLAE) with three-diagonal structure [8]. Let us note that the greatest effect of the parallel processor is reached by application of elements of the linear algebra for matrix computation.

Let us consider features of parallelization of SLAE with three-diagonal structures by the example of the solution of a test task for the heat conductivity equation.

Mathematical problem statetment.

Let us consider the solution of Dirichlet problem for the one-dimensional equation of heat conductivity

$$\frac{\partial Y}{\partial \boldsymbol{t}} = \alpha \frac{\partial^2 Y}{\partial \boldsymbol{x}^2}, \quad \boldsymbol{x} \in [\boldsymbol{x}_0, \boldsymbol{x}_L], \ \boldsymbol{t} \in [\boldsymbol{t}_0, \boldsymbol{T}] \quad (1)$$

with initial

$$Y_{|\ t=t_0} = \varphi(x) \quad (2)$$

and boundary conditions

$$Y_{|\ x=x_0} = YW(t), \ Y_{|\ x=x_L} = YL(t). \quad (3)$$

Let us compare net area to the area of determination of required function Y (t, x) in the tasks (1)-(3)

$$\left.\begin{aligned} t_j &= J \times Dt1, \quad j = \overline{1, M}, \qquad Dt1 = T / M, \ M \in Z \\ x_p &= p \times Dx1, \ \ p = \overline{0, 2m} \qquad Dx1 = (x_L - x_0) / 2m, m \in Z \end{aligned}\right\}, \quad (4)$$

Here, introduction of integer parameter *m* to topology of development of network nodes to the spatial variable *x* is used for solution of the task of vectorization of computation. It is required to solve the problem of the equation (1-3) discretization on the basis of the maximum parallel algorithm.

Statement of the main material of research

Let us consider a way of discretization of tasks (1)-(3) by method of finite differences [7 – 8].

The elementary implicit scheme by time and the central differences on coordinate *x* lead to SLAE

$$C_p Y_{p+1,1} - Y_{p,1} + D_p Y_{p-1,1} = f_{p,1}, \ \ p = \overline{1, 2m-1}, \quad (5)$$

where

$$\left.\begin{aligned} C_p &= D_p = \frac{A}{(1+2A)}, \ \ A = \frac{\alpha}{Dx1^2} Dt1 \\ f_{p_1} &= -\frac{YOp,1}{(1+2A)} \end{aligned}\right\}. \quad (6)$$

Here, the net functions

$$Y_{0,1} = fW(t_j), \quad Y_{2m,1} = fL(t_j),$$

contain information about boundary (3), and the right parts $f_{p,1}$ contain information about initial conditions, as net functions $YO_{p,1}$ are obtained from previous j-1-th time layer. Therefore, the numerical algorithm (5), (6) is evolutionary and consists in step-by-step change from one timepoint t_{j-1} to another one

$$t_j = t_{j-1} + Dt1 \cdot$$

For SLAE (5) with matrixes of form (6), there is an effective method of the solution – Gauss method of exclusion. This method is implemented by forward and backward sweep. Features of sweep are the small number of arithmetic actions and weak sensitivity to computing errors; these features make sweep be very convenient computing algorithm. However, this algorithm is resource and cannot be vectorized.

Among the known algorithms of recursive decomposition of the solution of band systems of equations, perhaps, only the algorithm of a cyclic reduction of shifts allows the highest level of vectorization. The idea of this algorithm consists in an exclusion of some coefficients of SLAE (5) by means of elementary conversions of lines. The conducted researches have shown that the procedure of elementary line conversions is possible only when an integer parameter value *m* is an even number in topology of network nodes (5). It has allowed us to establish global symmetry in relation to number *k* of the central node *m* and to formalize the procedure of elementary transformations of lines by method of "odd-even" reduction of lines of SLAE (5) in the parallel algorithm with the maximum extent of vectorization.

Computational algorithm

Stages of reduction of exclusion of variables with odd numbers, and further variables with even numbers {2,4,6,....}, {4,8,12,....}, etc., are implemented by means of binary constructions:

$$\left.\begin{aligned} Y_{p+2^{k-1},1} &= -f^{k-1}_{p+2^{k-1},1} + C^{k-1}_{p+2^{k-1}} Y_{p+2^k,1} + D^{k-1}_{p+2^{k-1}} Y_{p,1}, \\ Y_{p-2^{k-1},1} &= -f^{k-1}_{p-2^{k-1},1} + C^{k-1}_{p-2^{k-1}} Y_{p,1} + D^{k-1}_{p-2^{k-1}} Y_{p-2^k,1}, \end{aligned}\right\}, \tag{7}$$

where $k = 1,2,...$ – numbers in the order of a reduction.

In case of $k = 1$ we obtain:

$$Y_{p\pm1,1} = -f_{p\pm,1} + C_{p\pm,1} \begin{Bmatrix} Y_{p+2,1} \\ Y_{p,1} \end{Bmatrix} + D_{p\pm,1} \begin{Bmatrix} Y_{p,1} \\ Y_{p-2,1} \end{Bmatrix} \tag{8}$$

After substitution of variables $Y_{p\pm1}$ by means of ratios (8) in SLAE (5), we obtain SLAE of the same structure:

$$C^1_p Y_{p+2,1} - Y_{p,1} + D^1_p Y_{p-2,1} = f^1_{p,1} \tag{9}$$

In relation to variable with even numbers $\{Y_{2,1}, Y_{4,1},...Y_{2m-2,1}\}$, which are proportional to multiplicity 2.

Coefficients $C^1_p, D^1_p, f^1_{p,1}$ in (9) are calculated recurrently by formulas at $k = 1$:

$$\left.\begin{aligned} C^k_p &= \frac{C^{k-1}_p C^{k-1}_{p+2^{k-1}}}{Det_k}, \quad D^k_p = \frac{D^{k-1}_p D^{k-1}_{p-2^{k-1}}}{Det_k}, \\ f^k_{p,1} &= \frac{1}{Det_k}\left[f^{k-1}_{p,1} + C^{k-1}_p f^{k-1}_{p+2^{k-1},1} + D^{k-1}_p f_{p-2^{k-1},1} \right], \\ Det_k &= 1 - C^{k-1}_p D^{k-1}_{p+2^{k-1}} - D^{k-1}_p C^{k-1}_{p-2^{k-1}}, \end{aligned}\right\} \tag{10}$$

Where $C^0_p, D^0_p, f^0_{p,1}$ correspond to incoming data of initial SLAE (5). Repeated application of this process of reduction at $k = 2$ brings to

$$\left.\begin{aligned} Y_{p+2,1} &= -f^1_{p+2,1} + C^1_{p+2} Y_{p+4,1} + D^1_{p+2} Y_{p,1}, \\ Y_{p-2,1} &= -f^1_{p-2,1} + C^1_{p-2} Y_{p,1} + D^1_{p-2} Y_{p-4,1}, \end{aligned}\right\} \tag{11}$$

After substitution of variables $Y_{p\pm2,1}$ in (9), we obtain SLAE of three-diagonal structure:

$$C_p^2 Y_{p+4,1} - Y_{p,1} + D_p^2 Y_{p-4,1} = f_{p,1}^2 , \qquad (12)$$

where $p = \{4, 8, 12, ..., 2m-4\}$, i.e. proportional to 2^k, and data $\{C_p^2, D_p^2, f_{p,1}^2\}$ are calculated by formulas (10) at $k = 2$.

Repeated application of this process of reduction leads to SLAE of the same structure which generally takes the following form:

$$C_p^k Y_{p+2^k,1} - Y_{p,1} + D_p^k Y_{p-2^k,4} = f_{p,1}^k \qquad (13)$$

where $k = \overline{0, k_*}$ – numbers of reduction processes.

Thus, at the level of process of decomposition of SLAE (5), decomposition of all intermediate systems $\{C_p^k, D_p^k, f_{p,1}^k\}$ can be executed parallely and compensated with computation of variable of central node $Y_{m,1}$. Therefore, it is possible to claim that the developed algorithm possesses high degree of overlapping.

Conclusion

In an algorithm of "odd-even" reduction, many opportunities of multisequencing are hidden. Its application for the solution of three-diagonal systems on parallel computing systems is very relenant direction of applied mathematics. Its application is especially urgent for the solution of multivariate systems of the parabolic quasilinear equations describing processes of heat and mass exchange, i.e. for the decision of three-dimensional nonstationary tasks of heat conduction.

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