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DEVELOPMENT OF PARALLEL STRUCTURES OF DIFFERENTIAL TASKS OF MATHEMATICAL PHYSICS

The paper is devoted to the construction of parallel forms of mathematical models of a tridiagonal structure. Two methods of discretization of differential problems are considered by the example of solving the mathematical physics equation. Moreover, the application of the numerical-analytical straight line method and sweep methods to parallelization of mathematical models with a tridiagonal structure allows constructing its exact node-by-node solutions with the maximum parallel form and the least implementation time on parallel computing devices. This paper proposes to apply finite-difference and numerical-analytical methods in combination with the splitting method as a methodological basis for constructing numerical methods for solving such problems. The splitting method provides an economical and sustainable implementation of numerical models by the scalar sweep method. For such systems, acceptable acceleration in most cases is achieved by parallelizing operations in the corresponding sequential method, forming linear sections.

It is convenient to implement the parallelization algorithm and its mapping to parallel computing systems on the two schemes proposed in this paper: finite-difference and numerical-analytical. This approach allows arranging separate determination of the thermophysical characteristics of the structures' material, i.e. allows obtaining solutions of coefficient and other inverse problems of thermal conductivity.

The proposed approach to the development of methods, algorithms and software can be applied in various branches of metallurgical thermal physics, economics, as well as for environmental problems of the metallurgical industry.

Keywords: multiprocessor computing systems, mathematical models, parallel forms, thermal modes, sweep method, numerical-analytical method, tridiagonal structure

Introduction. A theoretical study of the process of heat and mass transfer is largely based on their numerical simulation using modern computer technology. However, with parallel computing tools development, fundamental problems disappear in a potentially infinite increase in their peak

performance. Parallel computing systems are developing very fast, and with the advent of computing clusters, parallel computing has become available.

To build such systems, as a rule, there is used mass processors, standard network technologies, and freely distributed software [1- 3]. It is these circumstances that allowed solving the so-called large problems of metallurgical thermophysics [4-6]. In metallurgical production, one faces many diverse and interconnected processes. Most of these processes (heat and mass transfer, hydrodynamic processes in melts, as well as a change in the state of substance aggregation, deformation phenomena under force and thermal loads, etc.) can be described on the basis of differential equations of continuum mechanics that reflect objective laws of the mass, momentum and energy conservation.

In mathematical terms, these are systems of multidimensional nonlinear differential equations, which along with the laws of chemistry and thermodynamics describe interrelated processes, as well as their interaction [7-9].

Modern computational methods and modern computers allow these days to carry out detailed parametric studies of mathematical models of very complex physical processes, or, as they often say, to conduct the so-called computational experiment.

Analysis of recent research and publications. Recently, in the theory and practice of studying various heat transfer processes, in thermal design and simulation of the thermal regimes of technical systems, a new direction of research has been intensively developing, based on principles of solving inverse heat transfer problems [10-13]. These methods were especially widely used in the experimental study of unsteady thermal processes accompanying the operation of heat-loaded aggregates and systems of space and descent aircraft, launch carriers, and various heat engines; in determining the thermo-physical characteristics of materials, building and adjusting mathematical thermal models of technical systems and in a number of other cases.

We note that at present the inverse problems of metallurgical thermophysics are formulated from the cause-effect relationships' point of view. Bringing them to extreme settings allows defining their solutions as optimal control problems. After defining direct mathematical models and introducing

the functional into the model according to the residual principle, the desired solution to various inverse problems is characterized only by unknown control parameters.

The usual results of a thermophysical experiment are now processed with respect to the requirements of statistics and the theory of scientific design of the experiment, since these results are statistical values. Currently, a simplified method for solving inverse problems of thermodynamics for non-stationary modes has been developed, which minimizes the functional for solving direct problems with minimizing many variables function. It is this circumstance that allows unifying the developed algorithms with regard to the causal characteristics of heat transfer processes and environmental dynamics in the problems of metallurgical thermophysics of ecology. To a large extent, this contributes to the integration of individual inverse problems solutions in the form of a set of programs.

The aim of the research is to construct the most parallel forms of mathematical models of a tridiagonal structure. The application of the numerical and analytical direct method and sweep methods for such systems parallelizing allow designing its solutions having the maximum parallel form and, therefore, the least time for its implementation on parallel computing devices.

The proposed approach to the development of methods, algorithms and programs is original and can be applied in various branches of metallurgical thermophysics, as well as environmental problems of the metallurgical industry.

Key research findings. Numerical simulation of heat and mass transfer processes is becoming increasingly important as modern science and technology require data on such processes, which experimental study in laboratory or field conditions is quite difficult and expensive, and in some cases simply impossible. This paper proposes application of finite-difference and numerical-analytical methods in combination with the splitting method as a methodological basis for constructing numerical methods for solving such problems. The splitting method provides with an economical and sustainable implementation of numerical models by the scalar sweep method. For such sys-

tems, acceptable acceleration in most cases is achieved by parallelizing operations in the corresponding sequential method, forming linear sections.

The adoption, as a methodological basis for differential problems discretization for difference splitting schemes of multidimensional spatial problems of the theory of heat and mass transfer, first of all, provides an economical and stable implementation of numerical models by the scalar sweeps method related to problems of linear algebra [10, 11]. And, secondly, it is known that the greatest effect of a parallel processor is achieved when it is used to perform linear algebra matrix computations [10].

Let us consider two methods of differential problems discretization by the example of solving the simplest scalar equation of mathematical physics:

$$\frac{\partial Y}{\partial t} = \alpha \frac{\partial^2 Y}{\partial x^2}, \quad x \in [x_0, x_L], t \in [t_0, T] \quad (1)$$

with initial

$$Y_{|t=t_0} = Y_0(x) \quad (2)$$

and boundary conditions of the first kind

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

The definition domain of the desired function is comparable to the net domain

$$t_j = j \cdot Dt, \quad j = \overline{1, M}, \quad Dt = T / M, \quad M \in \mathbf{Z},$$

$$x_p = p \cdot Dx, \quad p = \overline{0, 2m}, \quad Dx = (x_L - x_0) / 2m, \quad \mu \in \mathbf{Z} \quad (4)$$

The simplest implicit time scheme and central differences along the x coordinate lead to systems of linear algebraic equations (SLAE):.

$$C_P Y_{P+1,1} - Y_{P,1} + D_P Y_{P-1,1} = f_{P,1}, \quad p = \overline{1, 2m-1}, \quad (5)$$

wherein

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

In algorithm (5), (6) $Y_{0,1} = YW(t_j)$, $Y_{2m,1} = YL(t_j)$ are the known boundary functions, $YO_{p,1}$ is the initial vector function.

The SLAE (5) has a tridiagonal structure, and its solution is quite simply implemented recursively using direct sweep equations:

$$E_p = \frac{C_p}{1 - D_p E_{p-1}}, \quad G_p = \frac{D_p C_{p-1} - f_{p,1}}{1 - D_p E_{p-1}}, \quad (7)$$

wherein

$$E_0 = 0, \quad G_0 = Y_{0,1} = YW(t_y) \quad (8)$$

which ensures its start.

Inverse sweep equation:

$$Y_{p,1} = E_p Y_{p+1,1} + G_p, \quad Y_{2m,1} = YL(t_0) \quad (9)$$

is realized by index p from $p = 2m-1$ to $p = 1$.

This problem solution by the direct method also leads to SLAE (5), but with a different functional content:

$$\left. \begin{aligned} C_p &= \frac{S\eta\beta(1)}{S\eta\beta(2)} = D_p, \\ f_{p,1} &= C_p Y_{p+1,1}^* - Y_{p,1}^* + D_p Y_{p-1,1}^*, \end{aligned} \right\} \quad (10)$$

wherein $Y_{p+\varepsilon_x,1}^*$ ($\varepsilon_x = 0, \pm 1$) are particular solutions of the inhomogeneous equation:

$$Y_{p+\varepsilon_x,1}'' - \frac{1}{A} Y_{p+\varepsilon_x,1}(\varepsilon_x) = -\frac{1}{A} YO_{p+\varepsilon_x,1}(\varepsilon_x) \quad (11)$$

Note that here:

$$\varepsilon_X = \frac{x - x_p}{x_{p+1} - x_p} \in [-1, +1] \quad (12)$$

is the normalized spatial variable, $\alpha = \beta$ are the roots of the characteristic equation.

$$\beta^2 - \frac{1}{A} = 0 \quad (13)$$

The a priori information used in this case is a proposal for a piecewise - analytical dependence of the desired solution with respect to the spatial variable. Since the concretization of the form of a particular solution $Y_{p+\varepsilon_X,1}^*(\varepsilon_X)$ is inevitably associated with specific form of initial functions $YO_{p+\varepsilon_X,1}(\varepsilon_X)$ (11), when taking a quadratic dependence for them:

$$YO_{p+\varepsilon_X,1}(\varepsilon_X) = YO_{p,1} + \varepsilon_X YO_{p,2} + \varepsilon_X^2 YO_{p,3}, \quad (14)$$

wherein

$$\left. \begin{aligned} YO_{p,2} &= \frac{1}{2}(YO_{p+1,1} - YO_{p-1,1}) \\ YO_{p,3} &= \frac{1}{2}(YO_{p+1,1} - YO_{p-1,1} - 2YO_{p,2}) \end{aligned} \right\} \quad (15)$$

we see that the constructed solution becomes piecewise analytic on the entire set of p -nodes of the grid domain. The construction of particular solutions under this assumption is realized quite simply by standard methods.

Implementing the sweep algorithm by formulas (7) - (9), the solution of SLAE in the proposed formulation (10) - (15) allows defining values of net functions $Y_{p,1}$ in explicit form only as functions of a net node.

The above two schemes: finite-difference (5), (6) and numerical-analytical (5), (10) - (15) allows convenient implementation of an algorithm for parallelization and mapping onto parallel computing systems. In addition, this approach allows separate determination of the thermophysical characteristics of the structures' material, i.e. provides solutions to coefficient- and other inverse problems.

Conclusions and prospects for further research. The approach proposed in this paper for constructing parallel forms of mathematical models of a tridiagonal structure in the development of methods, algorithms, and programs is original and can be used in various branches of metallurgical thermophysics, as well as environmental problems of the metallurgical industry.

Moreover, the adoption as a methodological basis for discretization of multidimensional differential problems of split separation schemes, first of all, provides an economical and stable implementation of numerical models by the scalar sweeps method, and secondly, it is known that the greatest effect from a parallel processor is achieved when it is applied to perform matrix computations of linear algebra.

The application of the numerical-analytical method of straight lines and sweep methods to parallelizing SLAE of a tridiagonal structure allows constricting its exact node-by-node solutions having the maximum parallel form and, hence, the least time for its implementation on parallel computing devices.

Further research should be aimed at studying the topology of the net areas. This will lead to parallelization of SLAE by permutations based on the “odd-even” reduction algorithm.

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Розробка паралельних структур диференціальних задач математичної фізики

Теоретичне дослідження процесів тепло - і масообміну значною мірою базується на їх чисельному моделюванні з використанням сучасних засобів обчислювальної техніки. Проте з розвитком паралельних засобів обчислювальної техніки зникають принципові проблеми в потенційно нескінченному збільшенні їх пікової продуктивності. Для побудови таких систем, як правило, використовується масові процесори, стандартні мережеві

технології й вільно поширюване програмне забезпечення. Саме ці обставини й дозволили розв'язувати так звані великі задачі металургійної теплофізики.

Робота присвячена конструюванню паралельних форм математичних моделей трьохдіагональної структури. Класичні методи розв'язку математичних моделей трьохдіагональної структури при використанні багатопроцесорних обчислювальних систем обробляються, як правило, набагато повільніше, ніж при застосуванні однопроцесорної обчислювальної техніки. Ця обставина пояснюється рекурентним підходом, який покладений в основу класичних методів. В зв'язку з цим основна мета цієї роботи полягає в конструюванні максимально паралельних форм при моделюванні вказаного класу задач. На запропонованих в цій роботі схемах зручно реалізувати алгоритм розпаралелювання та його відображення на паралельні обчислювальні системи.

Такий підхід дозволяє організувати можливість роздільного визначення теплофізичних характеристик матеріалу конструкцій, тобто дозволяє отримати розв'язок коефіцієнтних та ін. обернених задач теплопровідності. В роботі розглянуто два способи дискретизації рівнянь математичної фізики. При цьому застосування числово-аналітичного методу прямих і методів прогонки до розпаралелювання математичних моделей, що мають трьохдіагональну структуру, дозволяє конструювати її точні повузлові рішення, що мають максимальну паралельну форму й мінімальний можливий час реалізації на паралельних обчислювальних пристроях.

Запропонований підхід при розробці методів, алгоритмів і програмних засобів може бути використаним в різних галузях металургійної теплофізики, економіки, а також задачах екології металургійної промисловості.

Development of parallel structures of differential tasks of mathematical physics

The paper is devoted to the construction of parallel forms of mathematical models of a tridiagonal structure. This paper considers two methods of discretization of differential problems on the example of solving the mathematical physics equation. Moreover, the application of the numerical-analytical straight-line method and sweep methods for parallelization of mathematical models with a three-diagonal structure allows constructing its exact node-by-node solutions having the most parallel form and the least implementation time on parallel computing devices. The proposed approach for the development of methods, algorithms, and software can be applied in various branches of metallurgical thermal physics, economics, as well as environmental problems of the metallurgical industry.

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