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Parallel Algorithms for Numerical Solution of Spatially Three-Dimensional Diffusion-Convection Equations in Coastal Systems Based on Splitting Schemes

Valentina V. Sidoryakina^{1,2} ✉, Denis A. Solomakha¹¹Don State Technical University, Rostov-on-Don, Russian Federation²Taganrog Institute named after A.P. Chekhov (branch) of RSUE, Taganrog, Russian Federation✉ cvv9@mail.ru

Abstract

Introduction. To prevent the occurrence and mitigate the consequences of hazardous and catastrophic phenomena associated with sediment transport in natural systems, it is necessary to develop operational and scientifically justified forecasts, identify critical states at which the emergence of emergency situations is possible. For these purposes, it is necessary to create an accurate and efficient toolkit, including algorithms for numerical solution of a model problem that takes into account the specifics of natural systems. In this work, parallel algorithms for numerical solution of a spatially three-dimensional diffusion-convection problem of sediment are presented, which allow a significant reduction in computation time (by more than 4 times) compared to calculations conducted using a sequential algorithm.

Materials and Methods. For the parallel solution of the spatially three-dimensional diffusion-convection problem, an implicit splitting scheme is constructed, in which the original continuous problem is replaced by a chain of two-dimensional and one-dimensional problems. The splitting schemes proposed in the work are physically justified and take into account the specifics of coastal marine systems, for which the influence of micro-turbulent diffusion and advective transport of substances are comparable, and the Peclet number does not exceed unity when approximating real problems. For the parallel numerical implementation, a method of decomposing the grid domain into two families of vertical planes parallel to the coordinate planes Oxz and Oyz , combined with the Seidel method for solving two-dimensional grid problems in horizontal planes and the tridiagonal matrix algorithm when solving one-dimensional three-point problems in the vertical direction, is used. Within the framework of the parallel computing software implementation, a parallel algorithm is presented that implements the diffusion-convection problem on a computing system using MPI technology.

Results. A comparative analysis of parallel and sequential algorithms is obtained using a model problem.

Discussion and Conclusions. The developed software allows its practical use for solving specific hydrophysical problems, including as part of a software complex.

Keywords: diffusion-convection problem, difference scheme, two-dimensional-one-dimensional scheme, parallel computing, Seidel method, tridiagonal matrix algorithm

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Параллельные алгоритмы численного решения пространственно-трехмерных задач диффузии-конвекции взвесей в прибрежных системах на основе схем расщепления

В.В. Сидорякина^{1,2} ✉, Д.А. Соломаха¹

¹Донской государственный технический университет, Российская Федерация, г. Ростов-на-Дону

²Таганрогский институт имени А.П. Чехова (филиал) РГЭУ (РИНХ), Российская Федерация, г. Таганрог

✉ cvv9@mail.ru

Аннотация

Введение. Для предупреждения возникновения и уменьшения последствий опасных и катастрофических явлений, связанных с переносом взвеси в природных системах, необходимо строить оперативные и научно оправданные прогнозы, выявлять критические состояния, при которых возможно появление чрезвычайных ситуаций. Для этих целей следует создать точный и быстро работающий инструментарий, включающий алгоритмы численного решения модельной задачи, учитывающей специфику природных систем. В настоящей работе представлены параллельные алгоритмы численного решения пространственно-трехмерной задачи диффузии-конвекции взвеси, позволяющие ощутимо снизить время расчёта (более чем в 4 раза), при сравнении с расчетами, проводимыми с использованием последовательного алгоритма.

Материалы и методы. Для параллельного решения пространственно-трехмерной задачи диффузии-конвекции построена неявная схема расщепления, в которой исходная непрерывная задача заменяется на цепочку двумерных и одномерных задач. Предлагаемые в работе схемы расщепления являются физически обоснованными и учитывают специфику прибрежных морских систем, для которых влияние микротурбулентной диффузии и адвективного переноса субстанций сопоставимы, причем при аппроксимации реальных задач сеточное число Пекле не превосходит единицы. Для параллельной численной реализации использован метод декомпозиции сеточной области двумя семействами вертикальных плоскостей, параллельными координатным плоскостям Oxz и Oyz , в сочетании с методом Зейделя при решении двумерных сеточных задач в горизонтальных плоскостях и методом прогонки при решении одномерных трехточечных задач по вертикальному направлению. В рамках программной реализации параллельного счёта представлен параллельный алгоритм, реализующий задачу диффузии-конвекции на вычислительной системе с использованием технологии MPI.

Результаты исследования. Получен сравнительный анализ параллельного и последовательного алгоритмов на примере решения модельной задачи.

Обсуждение и заключения. Разработанное программное средство позволяет его практически использовать для решения конкретных гидрофизических задач, в том числе в качестве элемента программного комплекса.

Ключевые слова: задача диффузии-конвекции, разностная схема, двумерно-одномерная схема, параллельные вычисления, метод Зейделя, метод прогонки

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Introduction. In numerical modelling of applied substance transport problems, convection-diffusion equations [1–4] serve as the foundation. The main features of such problems include, in particular, the non-self-adjointness of the problem operator, as well as significant differences in the spatial-temporal scales of the convective and diffusive transport difference operators [5–8]. These problem characteristics must be accounted for at the discrete level when constructing an approximation of the continuous problem.

When solving these problems numerically with a focus on efficient parallelization the perspective of efficient parallelization, the method of splitting along geometric directions has proven itself well [9–12]. The considered implicit scheme is based on splitting the three-dimensional diffusion-convection operator into two-dimensional and one-dimensional operators and forming a two-dimensional-one-dimensional additive splitting scheme. The solution of the difference three-dimensional problem reduces to solving a sequence of interconnected two-dimensional and one-dimensional difference problems based on initial and boundary data, which significantly reduces the time required for exchange operations in a parallel computing system. For the numerical solution of the two-dimensional difference diffusion-convection problem, a parallel variant of

the Seidel method is used, based on the decomposition of the three-dimensional grid problem by vertical planes parallel to the corresponding coordinate planes according to the number of parallel processors. The set of one-dimensional difference diffusion-convection problems in the vertical direction is solved in each processor independently of the others using a sequential tridiagonal algorithm. When using such an algorithm, the costs of interprocessor exchanges are significantly reduced compared to one-dimensional splitting schemes, which are performed according to the five-point template for boundary nodes included in separate blocks of grid information assigned for processing in individual processors. The approximation uses a skew-symmetric representation of convective terms, as well as the characteristics of flows in coastal marine systems, for which, in the vast majority of cases, the Peclet number does not exceed unity. This, in turn, allows for real problems when choosing a time step (seconds or a few tens of seconds) to ensure strict diagonal dominance in the matrix corresponding to the problem operator, and the convergence of the Seidel method at a geometric progression rate. A comparative analysis of parallel and sequential algorithms is carried out using a model problem.

Materials and methods

Difference scheme for the three-dimensional convection-diffusion equation. In the rectangular Cartesian coordinate system, let us consider the three-dimensional convection-diffusion equation using the skew-symmetric representation of the convective transport operator:

$$\frac{\partial c}{\partial t} + \frac{1}{2} \left[u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} + w \frac{\partial c}{\partial z} + \frac{\partial(uc)}{\partial x} + \frac{\partial(vc)}{\partial y} + \frac{\partial(wc)}{\partial z} \right] = \frac{\partial}{\partial x} \left(\mu_h \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu_h \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial z} \left(\mu_v \frac{\partial c}{\partial z} \right) + f, \quad (1)$$

where $c, c = c(x, y, z, t)$ is the concentration of particles at time $t, t \in [0; T]$; u, v, w are the components of the water medium velocity vector \vec{U} ; μ_h, μ_v are the coefficients of horizontal and vertical particle diffusion, f is the source function, $f = f(x, y, z, t)$.

The equation (1) is supplemented by initial conditions and Dirichlet boundary conditions:

$$c(x, y, z, 0) = c_0(x, y, z), \quad (x, y, z) \in \bar{G}, \quad (2)$$

$$\bar{G} = \{(x, y, z) | 0 \leq x \leq l_x, 0 \leq y \leq l_y, 0 \leq z \leq l_z\}, \quad \partial G = \bar{G} \setminus G;$$

$$c(x, y, z, t) = v(x, y, z, t), \quad 0 \leq t \leq T, \quad (x, y, z) \in \partial G. \quad (3)$$

Let's introduce a uniform rectangular space-time grid $\omega = \omega_h \omega_\tau$, where

$$\omega_h = \{x_i = ih_x, y_j = jh_y, z_k = kh_z, \quad i = \overline{1, N_x}, j = \overline{1, N_y}, k = \overline{1, N_z}, \quad N_x h_x = l_x, N_y h_y = l_y, N_z h_z = l_z\},$$

$$\omega_\tau = \{t_n = (n + \alpha/2)\tau, \quad \alpha \in \{0, 1\}; \quad n = 0, 1, \dots, N_t; \quad N_t \tau \equiv T\}.$$

On the time grid ω_τ we replace the problem (1)–(3) with a chain of two-dimensional-one-dimensional problem of the form:

$$\frac{\partial c^{(1)}}{\partial t} + \frac{1}{2} \left[u \frac{\partial c^{(1)}}{\partial x} + v \frac{\partial c^{(1)}}{\partial y} + \frac{\partial(uc^{(1)})}{\partial x} + \frac{\partial(vc^{(1)})}{\partial y} \right] = \frac{\partial}{\partial x} \left(\mu_h \frac{\partial c^{(1)}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu_h \frac{\partial c^{(1)}}{\partial y} \right) + f^{(1)}, \quad (x, y, z) \in G, \quad (4)$$

$$t_n < t \leq t_n + 0.5\tau, \quad n = 0, 1, \dots, N_t - 1,$$

$$c^{(1)}(x, y, z, 0) = c_0(x, y, z), \quad (x, y, z) \in G, \quad (5)$$

$$c^{(1)}(x, y, z, t_n) = c^{(2)}(x, y, z, t_n), \quad (x, y, z) \in \bar{G}, \quad n = 1, 2, \dots, N_t - 1; \quad (6)$$

$$\frac{\partial c^{(2)}}{\partial t} + \frac{1}{2} \left[w \frac{\partial c^{(2)}}{\partial z} + \frac{\partial(wc^{(2)})}{\partial z} \right] = \frac{\partial}{\partial z} \left(\mu_v \frac{\partial c^{(2)}}{\partial z} \right) + f^{(2)}, \quad (x, y, z) \in G, \quad (7)$$

$$t_n + 0.5\tau < t \leq t_{n+1}, \quad n = 0, 1, \dots, N_t - 1,$$

$$c^{(2)}(x, y, z, t_n + 0.5\tau) = c^{(1)}(x, y, z, t_n + 0.5\tau), \quad (x, y, z) \in \bar{G}, \quad n = 0, 1, 2, \dots, N_t - 1, \quad (8)$$

supplemented with the Dirichlet boundary conditions of the first kind form (3), $f = f^{(1)} + f^{(2)}$. In terms of the two-dimensional problem for the substance concentration function c the superscript (1) is used here, and for the one-dimensional problem — (2). The source function f is represented as $f = f^{(1)} + f^{(2)}$. In the further reasoning, we use an overline above the functions $c, f^{(1)}, f^{(2)}$ to denote their grid analogs.

$$\frac{\bar{c}^{n+1/2} - \bar{c}^n}{\tau} + \frac{1}{2} \left(u(x, y, z) \frac{\bar{c}^{n+1/2}(x + h_x, y, z) - \bar{c}^{n+1/2}(x - h_x, y, z)}{2h_x} + \right.$$

$$\begin{aligned}
 & + \frac{u(x+h_x, y, z)\bar{c}^{n+1/2}(x+h_x, y, z) - u(x-h_x, y, z)\bar{c}^{n+1/2}(x-h_x, y, z)}{2h_x} \Bigg) + \\
 & + \frac{1}{2} \left(v(x, y, z) \frac{\bar{c}^{n+1/2}(x, y+h_y, z) - \bar{c}^{n+1/2}(x, y-h_y, z)}{2h_y} + \right. \\
 & \left. + \frac{v(x, y+h_y, z)\bar{c}^{n+1/2}(x, y+h_y, z) - v(x, y-h_y, z)\bar{c}^{n+1/2}(x, y-h_y, z)}{2h_y} \right) =
 \end{aligned} \tag{9}$$

$$\begin{aligned}
 & = \frac{1}{h_x} \left(\mu_h(x+h_x, y, z) \frac{\bar{c}^{n+1/2}(x+h_x, y, z) - \bar{c}^{n+1/2}(x, y, z)}{h_x} - \mu_h(x, y, z) \frac{\bar{c}^{n+1/2}(x, y, z) - \bar{c}^{n+1/2}(x-h_x, y, z)}{h_x} \right) + \\
 & + \frac{1}{h_y} \left(\mu_h(x, y+h_y, z) \frac{\bar{c}^{n+1/2}(x, y+h_y, z) - \bar{c}^{n+1/2}(x, y, z)}{h_y} - \mu_h(x, y, z) \frac{\bar{c}^{n+1/2}(x, y, z) - \bar{c}^{n+1/2}(x, y-h_y, z)}{h_y} \right) + \\
 & + \bar{f}_1^n, \quad (x, y, z) \in \omega_h, \quad n = 0, 1, \dots, N_t - 1, \\
 & t^n < t \leq t^{n+1/2}, \quad n = 0, 1, \dots, N_t - 1,
 \end{aligned} \tag{10}$$

$$\bar{c}^1(x, y, z, 0) = c_0(x, y, z), \quad (x, y, z) \in \omega_h, \tag{11}$$

$$\bar{c}^n(x, y, z, t_n) = \bar{c}^{n+1/2}(x, y, z, t_n), \quad (x, y, z) \in \bar{\omega}_h, \quad n = 1, 2, \dots, N_t - 1. \tag{12}$$

The difference analogs of equations (7), (8) take the form:

$$\begin{aligned}
 & \frac{\bar{c}^{n+1} - \bar{c}^{n+1/2}}{\tau} + \frac{1}{2} \left(w(x, y, z) \frac{\bar{c}^{n+1}(x, y, z+h_z) - \bar{c}^{n+1}(x, y, z-h_z)}{2h_z} + \right. \\
 & \left. + \frac{w(x, y, z+h_z)\bar{c}^{n+1}(x, y, z+h_z) - w(x, y, z-h_z)\bar{c}^{n+1}(x, y, z-h_z)}{2h_z} \right) = \\
 & = \frac{1}{h_z} \left(\mu_v(x, y, z+h_z) \frac{\bar{c}^{n+1}(x, y, z+h_z) - \bar{c}^{n+1}(x, y, z)}{h_z} - \mu_v(x, y, z) \frac{\bar{c}^{n+1}(x, y, z) - \bar{c}^{n+1}(x, y, z-h_z)}{h_z} \right) + \\
 & + \bar{f}_2^{n+1/2}, \quad (x, y, z) \in \omega_h, \\
 & t_n + 0.5\tau < t \leq t_{n+1}, \quad n = 0, 1, \dots, N_t - 1, \\
 & c^{n+1}(x, y, z, t_{n+1/2}) = \bar{c}^{n+1/2}(x, y, z, t_{n+1/2}), \quad (x, y, z) \in \bar{\omega}_h, \quad n = 0, 1, 2, \dots, N_t - 1.
 \end{aligned} \tag{14}$$

Numerical solution of the two-dimensional problem (4)–(6) is carried out by the method of successive over-relaxation, while the one-dimensional problem (13)–(14) is solved by the tridiagonal matrix algorithm. It can be shown that for problems with a Péclet number not exceeding unity, the successive over-relaxation method converges geometrically with a convergence factor of 0.7–0.9 for real problems in the hydrophysics of coastal systems. Similarly, under these conditions, the tridiagonal matrix algorithm remains stable. Due to these properties, in this paper, we do not delve into detailed explanations for brevity.

Research Results. Parallel computing implementation. Within this work, a parallel algorithm has been developed to solve the three-dimensional convection-diffusion problem described by equations (10)–(14) using MPI technology. The parallel implementation involved techniques for decomposing grid domains for computationally intensive convection-diffusion problems, considering the architecture and parameters of the computing system. The decomposition of the computational two-dimensional domain was carried out along two spatial variables, x and y , and a decomposition along one spatial direction (one vertical coordinate) was also utilized. The parallel algorithm for solving the two-dimensional problem (10) is illustrated in Fig. 1.

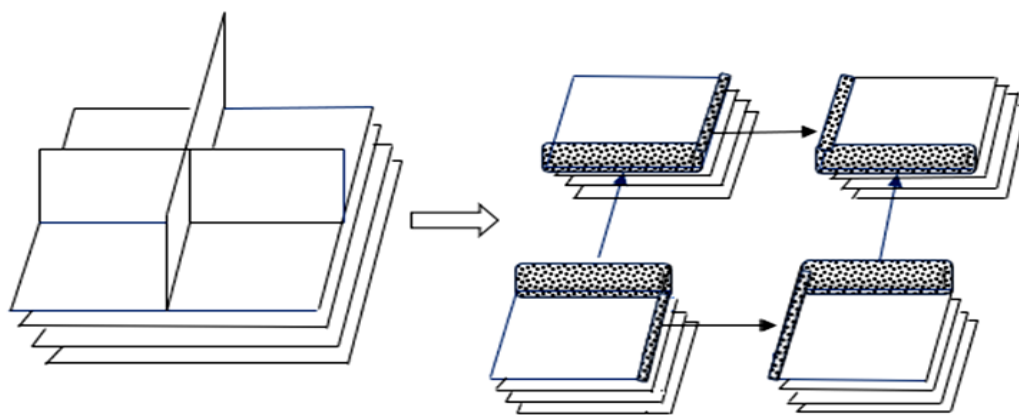


Fig. 1. Decomposition of the two-dimensional grid domain and the scheme for calculating the solution vector

Model Problem Solution. Let's demonstrate the results of the parallel algorithm's operation using a model problem for equation (1) with Dirichlet boundary conditions. The input data for the problem are as follows:

$$\begin{aligned}\vec{U} &= (u, v, w) = (x, 2y, 3 - 3z), \\ c &= k_1 x(l_x - x) + k_2 y(l_y - y) + k_3 \left(1 - \exp\left(-\frac{z}{l_z}\right)\right) + k_4(t + 0, 1), \\ \mu_h &\equiv \text{const}, \quad \mu_v \equiv k_5 \left(1, 1 + \sin\left(\frac{2\pi z}{l_z}\right)\right), \\ k_1 &= k_2 = 2x + l_x + 2y + l_y, \quad k_3 = \text{const}, \quad k_4 = \text{const}, \quad k_5 = \text{const}, \\ 0 &\leq t \leq 10, \quad l_x = l_y = l_z = 10 \text{ м}.\end{aligned}$$

Taking into account the specifics of coastal areas, coefficients k_3 , k_4 and k_5 of order 1÷5 were selected. Fig. 2 shows the dependency of the calculation time on the number of nodes in the computational grid for cases when parallel and sequential algorithms were used.

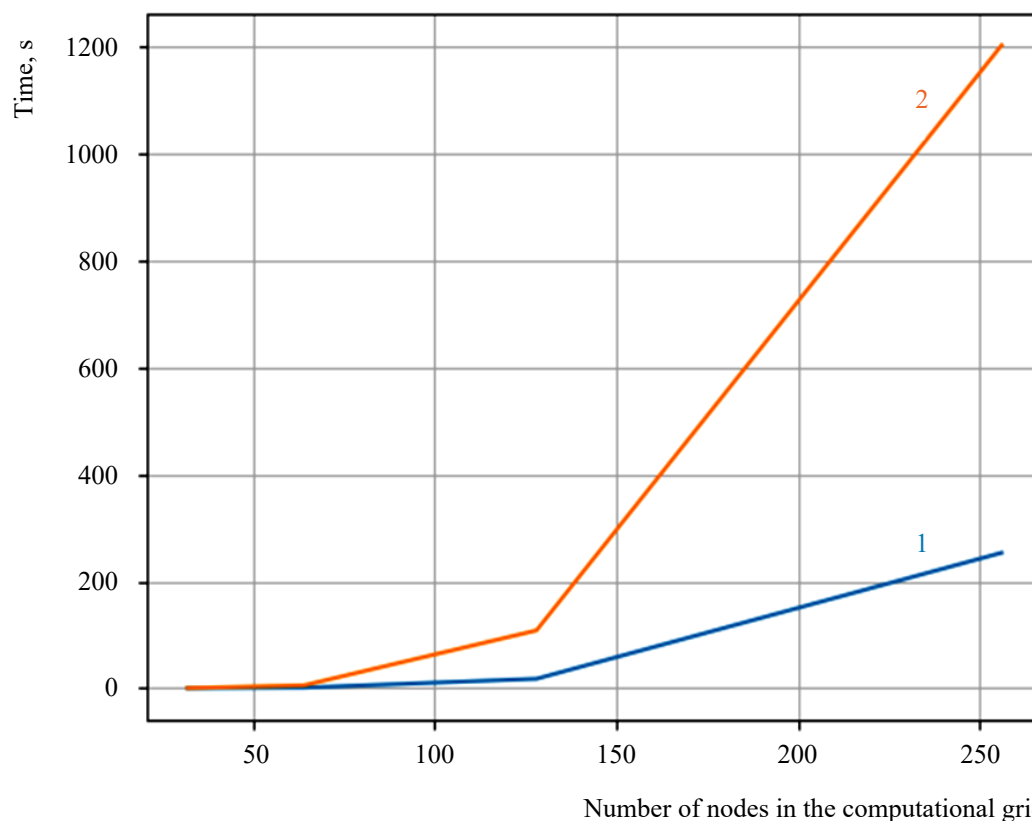


Fig. 2. Graphs depicting the dependence of calculation execution time on the number of nodes in the computational grid: 1 — for the parallel algorithm, 2 — for the sequential algorithm

Let's provide a comparative analysis of the calculation execution time (Table 1).

Table 1

Comparison of calculation execution time in the case of parallel and sequential algorithms

Number of Grid Nodes	32×32	64×64	128×128	256×256
Parallel Algorithm Execution Time, s	0.111	1.125	17.656	253.561
Sequential Algorithm Execution Time, s	0.388	5.405	108.180	1203.670

The results demonstrate a reduction in calculation time for the parallel algorithm by more than 4 times compared to the sequential algorithm.

Discussion and Conclusions. Algorithms for parallel and sequential computation have been proposed for solving the three-dimensional convection-diffusion problem. The application of the parallel algorithm can significantly reduce the calculation time (by more than 4 times), which is important for cases requiring timely risk analysis and determining the fate of suspended matter in the sea. The developed software tool enables practical use for solving specific hydrophysical problems, including as a component of a software complex. [11].

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About the Authors:

Valentina V. Sidoryakina, Associate Professor of the Department of Mathematics and Computer Science, Don State Technical University (1, Gagarin Sq., Rostov-on-Don, 344003, RF), Candidate of Physical and Mathematical Sciences, [MathSciNet](#), [eLibrary.ru](#), [ORCID](#), [ResearcherID](#), [ScopusID](#), cvv9@mail.ru

Denis A. Solomakha, 4th year student of the Department of Mathematics and Computer Science, Don State Technical University (1, Gagarin Sq., Rostov-on-Don, 344003, RF), [eLibrary.ru](#), solomakha.05@yandex.ru

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Об авторах:

Сидорякина Валентина Владимировна, доцент кафедры математики и информатики, Донской государственной технической университет (344003, РФ, г. Ростов-на-Дону, пл. Гагарина, 1), кандидат физико-математических наук, [MathSciNet](#), [eLibrary.ru](#), [ORCID](#), [ResearcherID](#), [ScopusID](#), cvv9@mail.ru

Соломаха Денис Анатольевич, студент 4 курса кафедры математики и информатики, Донской государственной технической университет (344003, РФ, г. Ростов-на-Дону, пл. Гагарина, 1), [eLibrary.ru](#), solomakha.05@yandex.ru

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