Software development for calculating the polluted by suspension and other impurities zones volumes on the basis of graphics accelerator

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Abstract. Software package construction for a distributed solution of the matter transfer problem in a reservoir is the aim of the work. The software package consists of several components that use different methods of interaction. The solution study posed by various methods and comparison of their performance is carried out. An algorithm for parallel solution on a graphics accelerator controlled by the CUDA system has been developed. A comparative analysis of the algorithms operation on CPU and GPU is carried out. The software implementation of the components included in the complex is described; the main classes and implemented methods are documented.

1. Introduction

Matter transfer mathematical modeling makes it possible to study the dynamics and trend of phenomena occurring in shallow water bodies and river systems [1]. It becomes possible to predict the anthropogenic interference consequences in the aquatic ecosystem.

The algorithms and programs development is necessary for the hydrodynamics model problems numerical implementation in coastal systems, including channel processes in river sections with the channel and floodplain complex morphometry [2]. This makes it possible to solve an important scientific and practical problem of assessing the planned technological facilities construction impact on the flooding of floodplain areas and the river bed erosion.

Abrasion is a result of the impact of channel flows destruction process. It is one of the factors that negatively affect the operation of the coast, various types of coastal structures and engineering equipment near river ports. The aquatic environment continuous movement leads to irreversible consequences, for example, to changes in the bottom topography, which occurs as a result of bottom sediments rise and transfer. Thus, the task of protecting the river systems coast infrastructure is important and urgent. It is necessary to build port and berthing facilities for the needs of the population of most settlements located on the banks of rivers. The construction and installation of coastal protection structures is an expensive and technically complex undertaking. One of the effective tools for analyzing and predicting the state of river systems is numerical modeling, which includes algorithms and programs development [3]. An important problem related to the river systems ecology is forecasting the spread of pollutants in the air and water environments.
The conducted research considers individual phenomena and does not cover them in a complex in the field of mathematical modeling of the processes of movement of pollutants in river systems, as well as in the development of numerical methods for solving problems [4-6]. It is necessary to develop and theoretically study new algorithms and programs for solving model problems, including the equations of aero- and hydrodynamics, satisfying the basic laws of conservation of matter, taking into account the multicomponent nature of the medium [7-8].

Currently, there is no universal method for constructing optimal three-dimensional computational grids [9]. Methods for constructing 3D unstructured grids for solving problems with discontinuous coefficients are described in detail in [10-12]. In [13-15], it was proposed to use the grid-characteristic method to solve this class of problems.

Since the tasks under consideration are complex and require large computing power, it is much more efficient to use parallel algorithms to perform calculations in the case of using a large amount of data. One of the ways to parallelize computations is to use CUDA technology, which allows to implement computations on a graphics accelerator.

2. Discrete mathematical model

The transfer problem is considered, it can be represented by the diffusion-convection equation [16]:

\[ c''(x, y, t) + uc'(x, y) + ve'(x, y) + f = 0 \]  

with boundary conditions:

\[ c'(x, y, t) = \alpha c(x, y, t) + \beta \]  

where \( u, v \) are the components of the velocity vector, \( \mu \) is the turbulent exchange coefficient, \( f \) is the function describing the intensity and distribution of sources.

The calculated area is inscribed in a rectangle. For the discrete mathematical model numerical implementation of the problem, a uniform grid is introduced [17]:

\[ w_h = \{ t^n = n\tau, x_i = ih_x = jh_y : n = 0, N_x, i = 0, N_y, \} \]

\[ N_x \tau = T, N_x h_x = l_x, N_y h_y = l_y \]

where \( \tau \) is the time step; \( h_x, h_y \) are space steps; \( l_x, l_y \) are the computational domain characteristic dimensions; \( N_x, N_y \) are boundaries in space; \( N_x \) is the upper time limit.

To approximate Eq. (1) in the time coordinate, we use schemes with weights

\[ \frac{\hat{c} - c}{\tau} + uc_x' + ve_y' = (\mu c_x')_x + (\mu c_y')_y + f \]

where \( c, \hat{c} \) are the values of the unknown function on \( n \) and \( n+1 \) time layers; \( e = \sigma \hat{c} + (1-\sigma)c,\sigma \in [0,1] \) is the weight of the scheme.

Discrete analogs of the convective and diffusion transfer operators in the case of partial fullness of the computational cells take the form:
\[ (q_0)_{i,j} \frac{\dot{c}_{i,j} - c_{i,j}}{\tau} + (q_1)_{i,j} u_{i+1/2,j} \frac{c_{i+1,j} - c_{i,j}}{2h_x} + (q_2)_{i,j} u_{i-1/2,j} \frac{c_{i,j} - c_{i-1,j}}{2h_y} + \\
+ (q_3)_{i,j} v_{i,j+1/2} \frac{c_{i,j+1} - c_{i,j}}{2h_y} + (q_4)_{i,j} v_{i-1/2,j} \frac{c_{i,j} - c_{i-1,j}}{2h_x} = (q_1)_{i,j} \mu_{i+1/2,j} \frac{c_{i+1,j} - c_{i,j}}{h_x^2} \\
- (q_2)_{i,j} \mu_{i-1/2,j} \frac{c_{i,j} - c_{i-1,j}}{h_x^2} - (q_3)_{i,j} \mu_{i,j+1/2} \frac{c_{i,j+1} - c_{i,j}}{h_y^2} + (q_4)_{i,j} \mu_{i,j-1/2} \frac{c_{i,j} - c_{i-1,j}}{h_y^2} \\
- (q_5)_{i,j} \mu_{i,j} \frac{c_{i,j} - c_{i-1,j}}{h_y^2} - (q_6)_{i,j} \mu_{i,j} \frac{c_{i,j} - c_{i-1,j}}{h_x^2} + (q_7)_{i,j} \mu_{i,j} \frac{c_{i,j} - c_{i-1,j}}{h_y^2} + (q_8)_{i,j} \mu_{i,j} \frac{c_{i,j} - c_{i-1,j}}{h_x^2} + (q_9)_{i,j} \mu_{i,j} \frac{c_{i,j} - c_{i-1,j}}{h_y^2} \\
(5) \]

where \( q_i, i = 0..4 \) are the control volumes fullness coefficients [2].

Discrete analogue (5) of equation (1) describes not only the change in the impurity concentration due to boundary sources, but also the complex geometry of the computational domain.

3. Development of algorithms for solving the transfer problem based on CPU and GPU

Parallel algorithm that implements the transfer problem (1), (2) based on a graphics accelerator controlled by the CUDA system [18] is presented in this paper, the results of the algorithm are compared with the classical implementation on the CPU. The data on the computational grids and the running time of the software components are presented in tables 1 and 2.

**Table 1.** Results of the CUDA algorithm

| № | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  |
|---|----|----|----|----|----|----|----|----|----|
| \( N_x \) | 10 | 20 | 50 | 100| 200| 500| 1000| 1000| 1000|
| \( N_y \) | 10 | 20 | 50 | 100| 200| 500| 1000| 1000| 1000|
| \( T \) | 1  | 2  | 5  | 10 | 50 | 50 | 100 | 500 | 1000|
| Time (sec) | 0.065| 0.072| 0.102| 0.092| 0.412| 1.570| 10.957| 79.292| 134.51|

**Table 2.** Results of the CPU algorithm

| № | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  |
|---|----|----|----|----|----|----|----|----|----|
| \( N_x \) | 10 | 20 | 50 | 100| 200| 500| 1000| 1000| 1000|
| \( N_y \) | 10 | 20 | 50 | 100| 200| 500| 1000| 1000| 1000|
| \( T \) | 1  | 2  | 5  | 10 | 50 | 50 | 100 | 500 | 1000|
| Time (sec) | 0.002| 0.004| 0.02| 0.15| 4.22| 37.78| 273.05| 1413.97| 2721.85|

Figure 1 shows the operation time dependence graph on the grid size for evaluating the algorithms on the CPU and GPU operation. Similar graph using a logarithmic scale is shown for clarity. Numbers 1-9 mark the computational experiments on the abscissa axis, carried out on various computational grids described earlier in tables 1 and 2. The operating times of the software components for the CPU and GPU are marked on the ordinate axis in seconds.

CUDA is ineffective for small grids (up to 100x100 computational nodes), according to figure 1. CPU reaches its maximum acceleration on 100x100 computational nodes, according to table 2, which allows the GPU to be used where the CPU is not so good. Using CUDA reduces the computation time by an order of magnitude in the case of large grids (1000x1000 computational nodes). The maximum value of the ratio of the running time of the algorithm that implements the set task of transferring matter in a
shallow reservoir on a graphics accelerator (GPU) to the running time of a similar algorithm on the central processing unit (CPU) was 24.92, which is achieved on a 1000x1000 grid size.

![Figure 1](image1.png)

**Figure 1.** Software components operating time based on CPU and GPU

4. Software implementation

When solving the problem of transferring substances (1), (2), when the input data of the source function is selected using the developed software package, an image of the contour graph representing the source function appears on the right panel. When all the necessary parameters are loaded and the «START» button is pressed, the calculation of the assigned task begins, as evidenced by the entry in the table of running tasks. Figure 2 shows the information about the launched task.

![Figure 2](image2.png)

**Figure 2.** Displaying task status
It is possible to suspend a task after it has started. In this case, the calculator will save the state in the storage and it will be possible to resume the task later. Figure 3 shows the panel's response to pressing the «Pause» button.

**Figure 3.** Task in the «Pause» status

After the task has been suspended, it is possible to continue the work of the software component by pressing the «Resume» button. Figure 4 shows the result of pressing the button.

**Figure 4.** Resumed task
The next stage is waiting for the completion of the program component and viewing the results. When the task is completed, the status changes to «Completed». Figure 5 shows the completed task.

![Completed task](image)

**Figure 5.** Completed task

When you click the «View» button, window with the result view of the program module in a graphical representation opens, and download the result as a text file. Figure 6 shows the result of clicking «View» button.

![The algorithm result](image)

**Figure 6.** The algorithm result
The «Save as file» button allows you to load a file with the results of calculations. Table 3 shows the contents of the loaded file.

**Table 3. The result file content**

|   | X1 | X2 | X3 | X4 | X5 | X6 | X7 | X8 | X9 | X10 |
|---|---|---|---|---|---|---|---|---|---|---|
| Y1| 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0   |
| Y2| 0  | 0.007891 | 0.022129 | 0.020214 | 0.015181 | 0.01128 | 0.004511 | 0.004543 | 0.001249 | 0  |
| Y3| 0  | 0.020942 | 0.044146 | 0.051694 | 0.029435 | 0.015595 | 0.012113 | 0.005559 | 0.002768 | 0  |
| Y4| 0  | 0.018931 | 0.049487 | 0.052433 | 0.030232 | 0.020525 | 0.012237 | 0.006177 | 0.004505 | 0  |
| Y5| 0  | 0.012748 | 0.027527 | 0.028419 | 0.024343 | 0.016913 | 0.009832 | 0.009109 | 0.001787 | 0  |
| Y6| 0  | 0.00944 | 0.013235 | 0.019048 | 0.015776 | 0.011665 | 0.010528 | 0.004581 | 0.003588 | 0  |
| Y7| 0  | 0.003928 | 0.009577 | 0.010572 | 0.009328 | 0.0096 | 0.006565 | 0.003376 | 0.003207 | 0  |
| Y8| 0  | 0.002681 | 0.005221 | 0.004688 | 0.007556 | 0.004782 | 0.002792 | 0.005524 | -0.000754 | 0  |
| Y9| 0  | 0.001425 | 0.00136 | 0.0039 | 0.001606 | 0.002635 | 0.003315 | -0.000883 | 0.002459 | 0  |
| Y10| 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0   |

The main functions of the developed software package, the functions of starting the calculation of the problem, viewing the results are tested in operation. The developed software is efficient, as evidenced by test calculations.

**5. Conclusions**

Much attention is paid to the study of transfer processes in practice. The processes taking place on the coastal areas with the adjacent water area often lead to a change in the shape of the bottom and the coastline. During the movement of sediments, three stages can be distinguished: the involvement of sediments from bottom sediments into movement, the movement of sediments, and the transition of moving sediments into bottom sediments. Building a general model of the movement of matter is a complex process. First, the individual process components are simulated. Then several models are combined into one.

In this work, software package focused on a graphics accelerator was implemented. The complex makes it possible to calculate the transfer problem in a shallow water body on various computational grids. The parallel algorithm implemented in the software package, oriented to the graphics accelerator, can significantly reduce the operating time of the software package with a large amount of input data. The presented complex is a distributed system with centralized control. It can be used to study aquatic ecosystems, assess the technogenic impact on them.

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