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THE COMPUTER WITH PARALLEL ARCHITECTURE IN A PROBLEM OF WIND TRANSPORT OF POLLUTANTS AT EMERGENCE

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ABSTRACT

The problem of a wind transport of pollutants in an atmosphere is considered. The algorithm for the solution of finite-difference equations by a method of splitting on physical processes is briefly described in view of an opportunity of concurrent execution of a program on supercomputer of the SKIF family. The specialized databases together with digital maps on emissions of pollutants in an atmosphere, on parameters of land surface, characteristics of polluting substances are used. Results of the solution of two demonstration problems are given: wind transport of burning products at forest fire and transboundary transport on Byelorussian region.

Key Words: Air Quality, Wind Transport, Computing System with Parallel Architecture, Forest Fire, and Transboundary Transport.

1. INTRODUCTION

The objectives of work are:

- Development of concurrent algorithm for problem of wind transport of pollutants for supercomputer SKIF realized on classical clusters from computing units of wide application.
- Productivity estimation of a supercomputer on two real problems: transport of pollutants at forest fire and transboundary transport on territory of Belarus.
- Development of experimental system for the operative forecast of wind transport of pollutants with use of GIS-technologies.

Mathematical models of wind transport of pollutants at emergence are described by significant number of the equations and variables that demands the massive capacities of used computers. In work the experimental program-information complex realized on distributed system from two computers is considered: PC (the cartographic module, input of parameters, visualization of results on maps) and supercomputer SKIF (calculating modules of problems on modeling of forest fire and transport of pollutants).

Many authors discussed the problem of pollutant transport in an atmosphere; see, for example, (Marchuk, 1982, Zlatev, 2002). It is necessary to solve system of the equations with partial derivatives

$$\frac{\partial c_s}{\partial t}+\frac{\partial (uc_s)}{\partial x}+\frac{\partial (vc_s)}{\partial y}+\frac{\partial (\tilde{w}c_s)}{\partial z}=$$

$$=K_x\left(\frac{\partial^2 c_s}{\partial x^2}+\frac{\partial^2 c_s}{\partial y^2}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial c_s}{\partial z}\right)+E_s-(k_{1s}+k_{2s})c_s\,, \qquad (1)$$

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0\,.$$

Here c_s - concentration of s-th pollutant, s = 1, 2, …, q; $\tilde{w}=w-w_s^g$; u, v, w – components of a wind velocity; w_s^g - velocity of gravitational sedimentation of s-th pollutant in an atmosphere; K_x, K_z - eddy diffusivity coefficients of air; functions E_s describe spatial sources of emissions of pollutant in an atmosphere, and k_{1s} and k_{2s} - coefficients of dry and wet deposition.

It is necessary to attach to the equations still corresponding initial and boundary conditions, in particular for imitation of pollutants emissions from a land surface.

2. THE BRIEF DESCRIPTION OF ALGORITHM

For the solving of the equations (1) the method of their splitting on physical processes is used, (Marchuk, 1982, Marchuk, 1989):

- *Transport of pollutants on trajectories* $\frac{\partial c_s}{\partial t}+\frac{\partial (uc_s)}{\partial x}+\frac{\partial (vc_s)}{\partial y}+\frac{\partial (\tilde{w}c_s)}{\partial z}=0;$ (2)
- *Eddy diffusivity of pollutants* $\frac{\partial c_s}{\partial t}=K_x\left(\frac{\partial^2 c_s}{\partial x^2}+\frac{\partial^2 c_s}{\partial y^2}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial c_s}{\partial z}\right)$**;** (3)
- *Interaction of pollutants sources* $\frac{\partial c_s}{\partial t}=E_s-(k_{1s}+k_{2s})c_s$**.** (4)

For numerical integration of the equations (2) the two-cyclic implicit finite-difference scheme of the second order of the accuracy was used. For the sake of simplicity the index s at a variable c is omitted, h - step of a grid on x and y, $\{\Delta z_{n+1/2}\}$ - steps of a grid on z, $\tau=\frac{1}{2}(t_{j+1}-t_j)$, $u_{k+1/2}=\frac{1}{2}(u_{k+1}+u_k)$, $v_{m+1/2}=\frac{1}{2}(v_{m+1}+v_m)$, $\tilde{w}_{n+1/2}=\frac{1}{2}(\tilde{w}_{n+1}+\tilde{w}_n)$, $\Lambda_1^j\varphi=\frac{u^j_{k+1/2}\varphi_{k+1}-u^j_{k-1/2}\varphi_{k-1}}{2h}$, $\Lambda_2^j\varphi=\frac{v^j_{m+1/2}\varphi_{m+1}-v^j_{m-1/2}\varphi_{m-1}}{2h}$,

$\Lambda_3^j \varphi = \dfrac{\tilde{w}_{n+1/2}^j \varphi_{n+1} - \tilde{w}_{n-1/2}^j \varphi_{n-1}}{\Delta z_{n+1/2} + \Delta z_{n-1/2}}$, $E\varphi = \varphi$ - identity operator. Those indexes that differ from k, m, n on only ±1 are written out.

First cycle *Second cycle*

$$\left(E + \frac{\tau}{2}\Lambda_1^j\right)c^{j+1/6} = \left(E - \frac{\tau}{2}\Lambda_1^j\right)c^j, \qquad \left(E + \frac{\tau}{2}\Lambda_3^j\right)c^{j+4/6} = \left(E - \frac{\tau}{2}\Lambda_3^j\right)c^{j+3/6},$$

$$\left(E + \frac{\tau}{2}\Lambda_2^j\right)c^{j+2/6} = \left(E - \frac{\tau}{2}\Lambda_2^j\right)c^{j+1/6}, \qquad \left(E + \frac{\tau}{2}\Lambda_2^j\right)c^{j+5/6} = \left(E - \frac{\tau}{2}\Lambda_2^j\right)c^{j+4/6}, \qquad (5)$$

$$\left(E + \frac{\tau}{2}\Lambda_3^j\right)c^{j+3/6} = \left(E - \frac{\tau}{2}\Lambda_3^j\right)c^{j+2/6}, \qquad \left(E + \frac{\tau}{2}\Lambda_1^j\right)c^{j+1} = \left(E - \frac{\tau}{2}\Lambda_1^j\right)c^{j+5/6}.$$

The equations of eddy diffusivity (3) are solved by traditional method of splitting on spatial variables and one-dimensional factorizations, and the system (4) can be treated in each point of integration domain as system of the ordinary differential equations, in which coefficients depend on spatial variables as parameters.

The considered problem demands knowledge of a wind field and eddy diffusivity coefficient $K_z(z)$ in a boundary layer of an atmosphere. For their calculation we used the Monin-Obukhov's *K*-ε theory of similarity which realization is described in (Yordanov et al., 2002).

The problem possesses by natural parallelism: calculation of concentration of each impurity can be conducted on the separate processor, reducing due to it time of calculations almost in *q* time, where *q* - number of impurity (several tens).

Primary parallelisation is done on pollutants when calculation of *q* impurities was distributed on *P* processors of a supercomputer. If the number of processors *P* is more than number of considered pollutants *q* calculation of impurity it is possible to divide on *P/q* concurrent streams. This internal parallelisation uses splitting the general three-dimensional problem on a series of one-dimensional problems. Calculation is done in four consecutive stages.
1-*st stage* – transport of substances on trajectories (the first cycle of finite-difference scheme):

- (*M*-1) · (*N*-1) simultaneous factorizations on *x*,
- then (*K*-1) · (*N*-1) simultaneous factorizations on *y*,
- then (*K*-1) · (*M*-1) simultaneous factorizations on *z*.

2-*nd stage* - transport of substances on trajectories (the second cycle of finite-difference scheme):

- again (*K*-1) · (*M*-1) factorizations on *z*,
- (*K*-1) · (*N*-1) factorizations on *y*,
- (*M*-1) · (*N*-1) factorizations on *x*.

3-*rd stage* – diffusion of pollutants:

- (M-1) · (N-1) simultaneous factorizations on x,
- then (K-1) · (N-1) simultaneous factorizations on y,
- then (K-1) · (M-1) simultaneous factorizations on z.

For example, factorizations on z are shown on Figure 1.

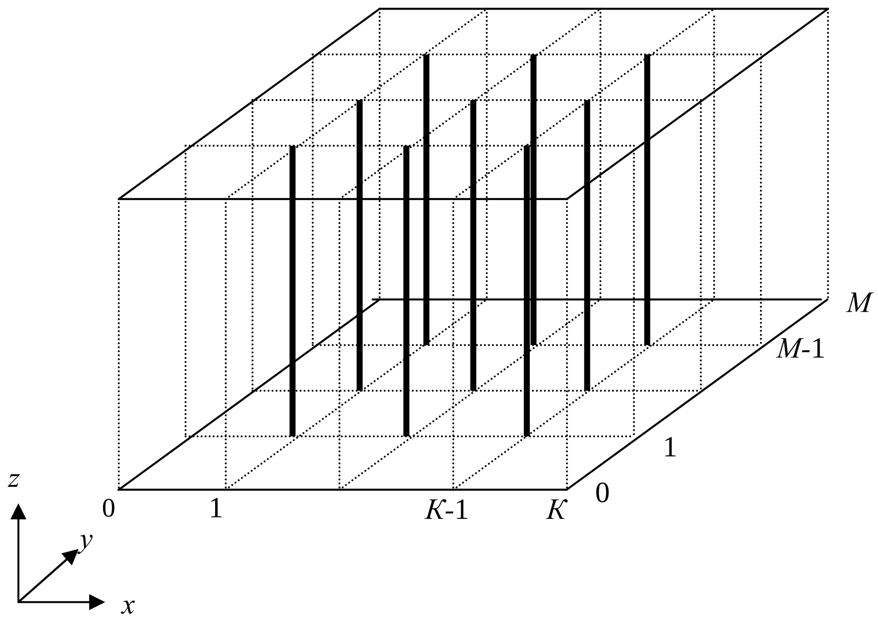

Figure 1. Organization of concurrent calculations in one direction

It is possible to note one more kind of parallelism inherent in the considered method of the program execution. Apparently from (5), all calculations break up to separate one-dimensional factorizations. For example, factorizations in a vertical direction can be carried out simultaneously in all points (K-1) (M-1) a land surface (Figure 1). If, for example, number of nodes K = 31 and M = 31, it is potentially possible to speed up calculations almost in 900 times. However, thereof that number of accessible processors are less than 900, the service of simultaneous factorizations are necessary to organize specially. It would be interesting to carry out experiment with an estimation of an arising overhead charge in this case.

3. AN EXPERIMENTAL COMPLEX

The problem was solved on the two-machine complex consisting of terminal personal computer Pentium 4 and supercomputer K-500 of the SKIF family (Ablamejko and Abramov, 2003). The PC was used for preparation of the initial data (meteorological, cartographic and on emissions of pollutants in an atmosphere), for management of calculations on a two-machine complex and processing of results (drawing of pollution maps of territory and their storage). The supercomputer was used as the powerful calculator for the numerical tasks prepared on the personal computer.

Family of supercomputers SKIF. The basic principles of family of supercomputers (open scaled architecture, a set of base computing modules and configurations, etc.) allow optimum way to create an adequate supercomputer configuration for each concrete applied problem. The key features of supercomputer SKIF are done in Table 1.

Table 1. The SKIF key features

Attribute	*Characteristic*
Scope	Scientific and engineering calculations
Type of a computer	Cluster
Peak productivity	2 534,4 Gflops
Operating system	Linux SUSE Linux Enterprise Server 8 + SP3
Amount of processors	576
Total volume of operative memory	1 152 Gb
Total volume of disk memory	23 040 Gb
Amount of nodes	288
Number of processors on node	2
The firm-manufacturer of the processor	AMD
Type of the processor	Opteron 248
Clock frequency of the processor	2 200 MHz
Operative memory on node	4 000 Mb
Disk memory on node	80 Gb
Communication network	InfiniBand
Transport network	Gigabit Ethernet
Service network	SKIF – ServNet

The SKIF K-1000 is the superior model of family. As the much as possible reached productivity on the test Linpack is 2 032 Gflops for a matrix by a size of 274 000 units. The supercomputer model SKIF K-1000 inscribed in the list of 500 most productive computers of a world in 2004 (http://www.top500.org).

4. THE CARTOGRAPHIC MODULE

All results of the calculations are processed and displayed by cartographic system (Kruchkov et al., 2003) on a digital map of district. The cartographic system uses as the initial data the digital maps of Belarus and the adjoining regions in scale 1:500000 and 1:100000.

The output of cartographic system and a complex as a whole comprises the map of analyzed territory with results of modeling as fields of concentration and isolines on a map and a legend of a thematic map (levels of concentration, a drawing scale, conventional signs, the text).

5. THE DEMONSTRATION TASKS

Two demonstration tasks were solved: the FIRE - the forecast for several days the spread of the pollutants arising at forest fire, and TRANS - calculation of pollution of Belarus territory by the substances which are starting with some ground sources within 30 days.

In the first task as sources of the pollutants acting in an atmosphere, the centers of forest fires on the territories of Belarus fixed in space pictures 11.09.2002 in Northeast of Byelorussia (Figure 2) were considered.

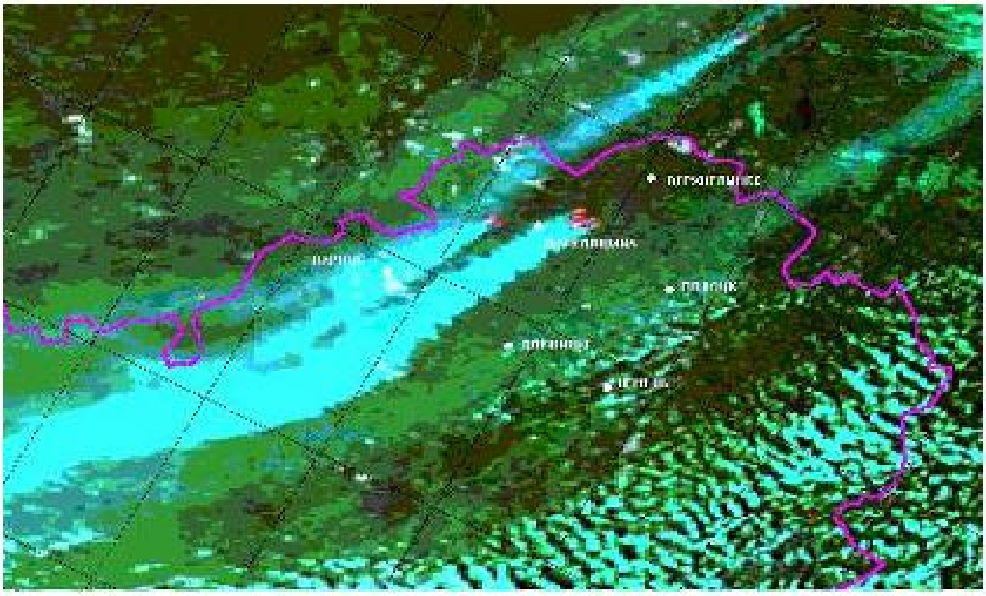

Figure 2. A snapshot of a forest fire in Northeast of Belarus

The coordinates of a fire were taken from a snapshot by means of a special measuring complex and were entered into a program through the personal computer. The quantity of burning products emitted for an elementary step on time was determined by a method, described in (Technique, 2002), and calculation of wind transport - by the way described in article. Concerning a land surface it was necessary to know its type (a forest, a field, a combustible land surface whether or not), absorption coefficient of pollutants dropping out on the ground, a specific output of burning products, a degree of land pollution by radionuclides and some other. The main part of these data was taken from a digital map of district, and also from special-purpose databases.

Meteorological data (approximately 5-6 parameters) were acquired from the meteorological station nearest to place of a forest fire.

The example of calculation of wind transport of smoke aerosol for 18 hours is resulted on Figure 3: on it the field of volumetric concentration of a smoke aerosol at height of 20 m is shown. To this time the smoke was disseminated to distance more than 30 km.

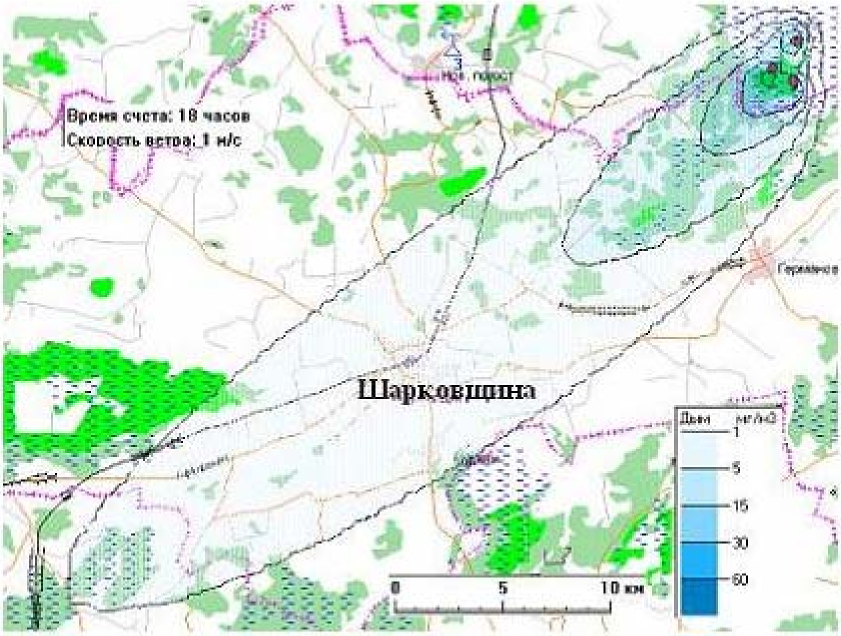

Figure 3. Transport of smoke at the forest fire

In the second task the field of wind velocity was set as follows. In eight base points of the meteorological observations placed on territory of Byelorussia the vertical profiles of velocity were calculated, starting from average climatic values for one month (Climate, 1996, Hand-book, 2003). Then the spatial fields of a wind in all grid points were defined on these profiles by the method of interpolation. As the permanent sources of emissions of pollutants in an atmosphere, 14 cities of Byelorussia have been considered, each of which throws out more than 2000 tons of impurities per year (Environment, 2001). On emissions it was necessary to know their sources, structure of emissions, a mode of functioning, sedimentation velocity of pollutants, etc. Nine impurities participated in calculations: solid particles (dust), CO, SO_2, NO_2, phenol, H_2CO, NH_3, CH, H_2S.

The transboundary transport of pollutants on territory of Byelorussia for 30 days within June, 2003 is shown on Figure 4. Volumetric concentration of all pollutants was calculated, and in Figure 4 isolines normalized concentration of CO is shown at height 500 m after 9 hours of modeling time. The normalized concentration is defined as $c_{norm} = \frac{c(x, y)}{\max(c)}$.

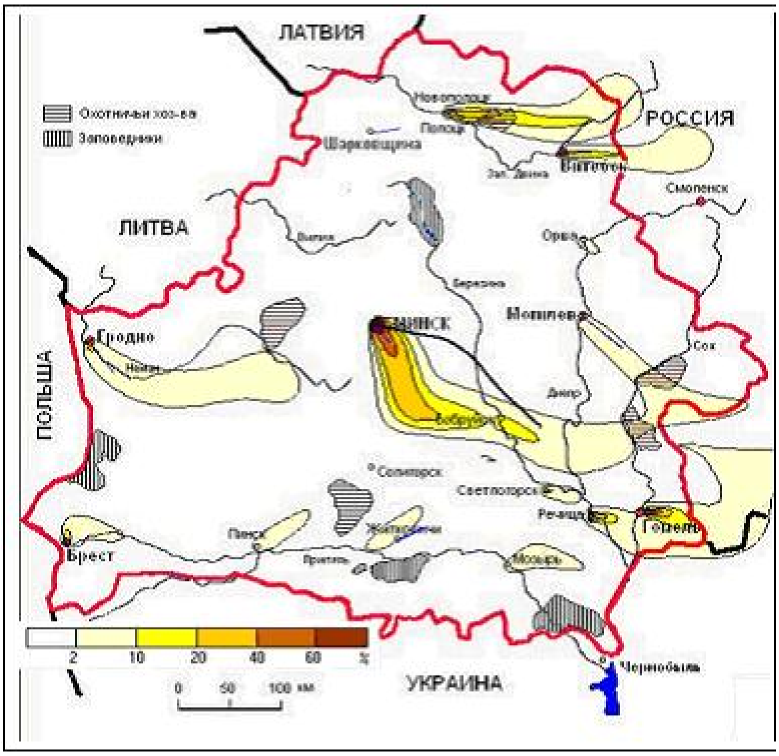

Figure 4. Transboundary transport of pollutants within a month. Horizontal and vertical shading marks the hunting facilities and reserves.

6. INTERCOMPARISON OF METHODS

For an estimation of accuracy of obtained results the special calculations on our program, on a technique adopted in USSR (Technique, 1987), and on a technique of Environmental Protection Agency of USA (U.S. Screening, 1988) were carried out.

The model, offered us, (we shall referred it "UIPI") is based on a numerical solution of the equations of mathematical physics well enough describing a continuous medium. At the same time, it is possible to expect an incongruity of our outcomes of simulation with outcomes OND and American in a neighbourhood of point sources of ejection owing to not enough their precise approximating at replacement of the differential equations of a continuous medium by the finite-difference equations for numerical calculations.

We examined an example from (Technique, 1987) about atmospheric emission SO_2 from single smoke-stack by height 35 m. Figure 5 shows the graphs of concentration $c(x)$ on axis of emission plume near land surface down wind, obtained by the models OND, SCREEN, and UIPI. The Figure displays, that the results of models UIPI and OND are well consisted with themselves: the location of the concentration peaks coincide, both maximal values coincide, and the graphs practically have the identical form.

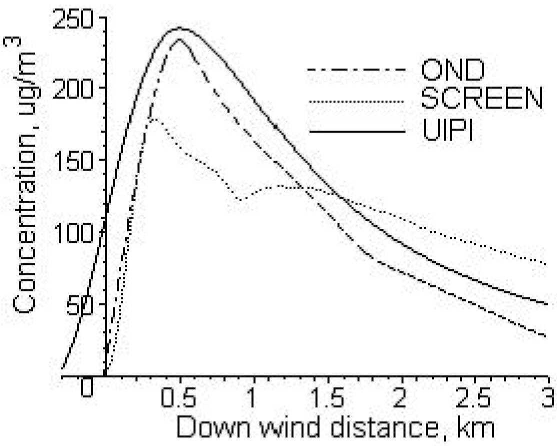

Figure 5. Intercomparison of methods

7. CONCLUSION

In Table 2 the execution time for demonstration tasks for supercomputer SKIF is resulted.

Table 2. Time of the task execution

Number of pollutants *N*	*N* pollutants on *N* processors	*N* pollutants on one processor	Acceleration
Forest fire for one day			
N = 4	10.2 min..	37 min.	3.6
Transboundary transport on 30 days			
N = 9	9.3 hours	56.1 hours	6.0

It is visible, what even the simplest parallelisation on pollutants results execution of demonstration tasks in significant acceleration of computing process. The developed program-information complex can be assumed as a basis system of the operative forecast of wind transport of pollutants at emergency situations.

The results, obtained on model UIPI, well enough coincide outcomes of a state technique OND, adopted at problem wind transport of pollutant in former USSR.

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