A Numerical Prediction of Urban Air Quality on Multiprocessor Computer Systems

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Introduction

Currently a monitoring of air pollution dispersion through urban atmosphere are exercises both instrumentally [1] and using numerical models. To correctly predict spatial distribution of gaseous and aerosol pollution incoming with industrial and vehicle emissions into atmosphere, it is necessary to apply models, which taking into account wind transport of substance, turbulent dispersion and chemical transformation. The most detailed pattern of atmospheric processes can be calculated on the basis of three-dimensional prognostic mesoscale models in combination with running assimilation of observation data [2,3].

In this paper a prediction of transport of air emissions injected elevated point sources, surface areal sources and urban vehicles is realized on the basis of Eulerian model of atmospheric diffusion. A short-term (one-two days) forecast of urban air quality is ensured by application of high performance computer systems and parallel programming technologies.

A Model of Pollution Transport

Prognostic equations of "advection-diffusion" type for small compounds of atmosphere are used to predict transport, dispersion and chemical transformation of air pollution:

$$\frac{\partial c_j}{\partial t}+\frac{\partial Uc_j}{\partial x}+\frac{\partial Vc_j}{\partial y}+\frac{\partial W_j c_j}{\partial z}=\frac{\partial}{\partial x}\left(K_Z^h\frac{\partial c_j}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_Z^h\frac{\partial c_j}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_Z^h\frac{\partial c_j}{\partial z}\right)+Q_j, j=1,...,s\,. \quad (1)$$

Here c_j is the concentration of j-th compound of admixture; Q_j is the source term, modeled incoming of admixture from emission sources and transformation of composition during photochemical reactions; U, V are the horizontal components of wind; W_j is the vertical velocity of j-th compounds of admixture; s is the number of admixture compounds; K_Z^h is the turbulent diffusivity. Simple boundary conditions ($c_j=0$ or $\frac{\partial c_j}{\partial n}=0$) are used.

A wind field and turbulent structure of atmosphere are predicted using an unsteady non-hydrostatic three-dimensional model of hydro- thermo- dynamics of atmosphere, based on conservation equations in differential form [2]. Problem of turbulent closure is solved by application of Boussinesq gradient relations in transport equations and two-equation turbulence model included prognostic three-dimensional equations for turbulent energy and turbulent scale.

Numerical Method

The problem of simulation of dynamic and thermal state of an urban atmosphere for selected temporal interval is solved numerically by finite-differencing method on a grid refined to surface. A compression of grid is assigned so that ratio of vertical sizes of adjoining grid cells would be constant. The first calculation level above surface greatly exceeds surface roughness parameter z_0. Horizontal dimensions of the differencing grid are constant. Discrete analogs of governing equations are constructed by finite volume method with the second-order temporal and spatial approximations. The obtained systems of differencing equations are solved by

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Buleev's explicit method of incomplete factorization. SIMPLE (Semi-Implicit Method for Pressure-Linked Equation) algorithm [4] is used for adjustment of velocity and pressure fields.

The unsteady, spatial equations (1), modeling transport of admixture compounds through the nested computational domain, are numerically integrated after solution of the main problem connected with prediction of velocity fields and turbulent structure of atmosphere. Approximations of differential operators in (1) are realized with the second order for spatial derivatives and first order for temporal derivatives. Explicit differencing scheme for equation (1) allows to resolve non-linearity problems and to speed up computations at acceptable limitation on time step. The advective terms of the prognostic equation (1) are approximated using Van Leer's monotonized linear upstream scheme, which doesn't allow appearance of negative values of concentration.

Prediction of Pollution Transport on Multiprocessor Computer Systems

In the developed modeling system of atmospheric processes and pollution transport the main computational loading is connected with a numerical solution of 3D prognostic equations (1). It is conditioned by necessity of application of high-density computational grid for urban conditions and consideration of the large number of chemical compounds to correctly simulate generation of secondary pollutants (for example, ozone). Therefore high performance computers (multiprocessor cluster systems of Tomsk State University (http://cluster.tsu.ru) and Institute of Atmospheric Optics (http://cluster.iao.ru)) are used to performing of numerical predictions. These systems are working in MPI standart (Message Passing Interface).

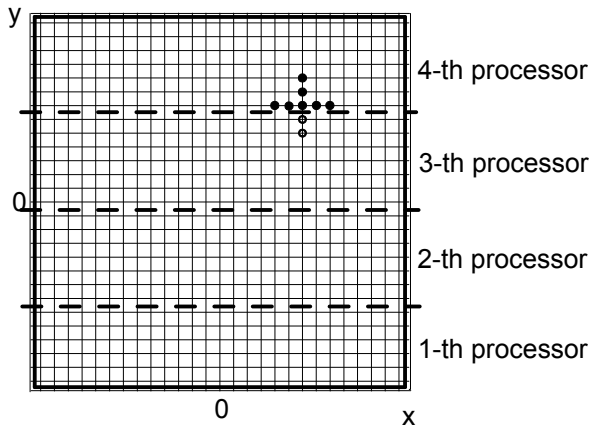

Fig.1. Computational grid in a plane xOy with indication of distribution of subdomains on four processors. A differencing stencil is shown in near boundary line. Open circles correspond to grid values, which should be received from adjoining processor

Parallel realization of numerical method of solution of equation (1) is performed on the basis of geometric principle – data decomposition [5]. A computational domain is divided on equal subdomains. In this paper a parallelepiped of computational domain $(-L_x/2 \le x \le L_x/2;\ -L_y/2 \le y \le L_y/2;\ \delta(x,y) \le z \le L_z;\ \delta(x,y)$ is the function, modeling relief of a surface) is cut by sections $y = \text{const}$ with distribution of subdomain data to corresponding processor element. Grid values of concentration $(c_j)_{k,l,m}^{n+1}$ are evenly distributed through computational nodes of multiprocessor system with distributed memory. Within each subdomain the discrete equations are simultaneously solved by TDMA algorithm. However, because of adopted differencing stencil (Fig.1), grid values of concentration from adjoining subdomain are necessary when we calculate concentration in nodes of two near boundary grid lines (near upper and bottom boundaries of a subdomain). Therefore inter-processor data exchange is realized with usage of MPI-function MPI_SendRecv.

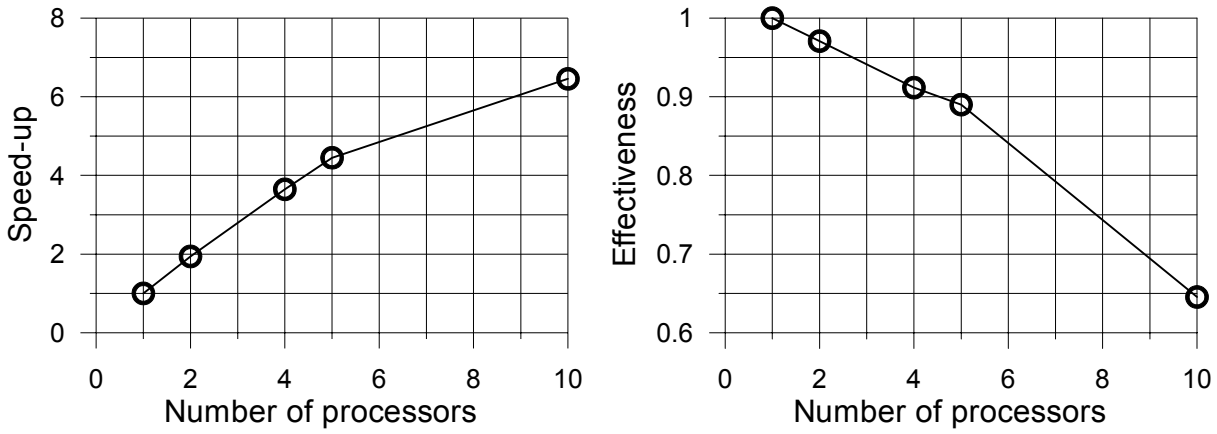

Fig.2. Speed-up and effectiveness of developed parallel algorithm.

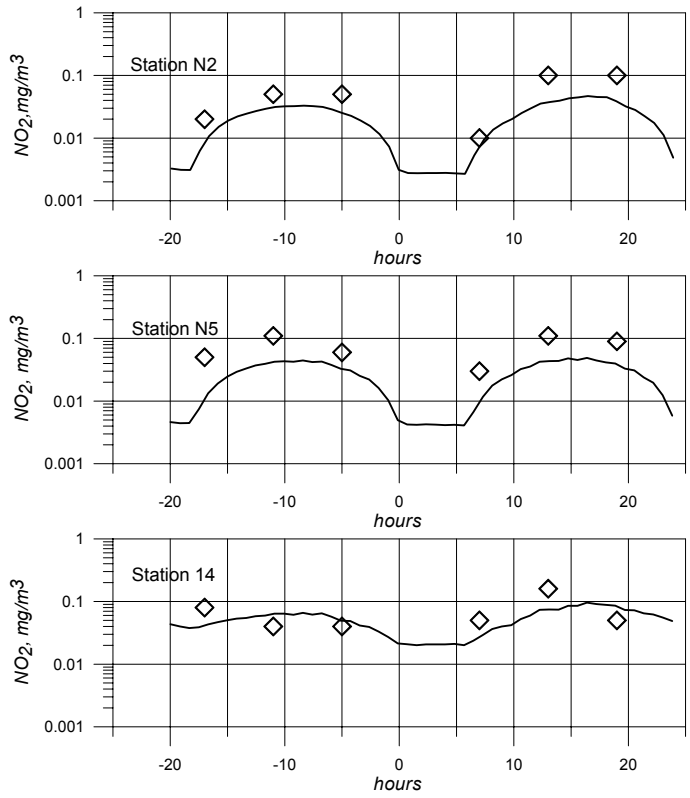

Fig.3. Concentration of nitrogen dioxide near Tomsk stations of air quality monitoring during 10 and 11 January 2000. Close circles correspond to measurements. Solid line is prediction

Developed modeling system was applied to prediction of distribution of basic urban pollutants (dust, CO, SO_2, NO_2) above Tomsk city. 119 linear, 12 areal and 338 point emission sources were considered in computations. Prediction of atmospheric parameters was performed on grid 50x50x30 for time step 60 sec. A grid 100x100x50 with time step 15 sec was used for post-computations of pollutant distribution through urban atmosphere.

Fig. 2 shows speed-up and effectiveness of above described parallel algorithm, obtained on TSU cluster system (9 double-processor computational nodes Pentium III 650MHz, RAM 256Mb, Fast Ethernet 100Mbit). In calculations speed-up is a ratio of CPU time of problem solution on single-processor computer to CPU time of problem solution on p-processor computer system at the fixed other parameters. Effectiveness is ratio of speed-up to number of processors used in calculations. From Fig.2 one can see that CPU costs can be reduced more than 6 times.

Effectiveness slowdown in dependence of using processor number is consequence of growth of inter-processor exchange with regard to computational work.

The predicted and measured values of nitrogen dioxide for conditions of 10-11 January 2000 are presented on Fig.3. On the whole, results of comparison should be admitted as satisfactory. More low values of predicted concentration of NO_2 are explained by used computational technology, which presents data averaged on grid cell (in computations it is parallelepiped with dimensions 500m:500m:20m).

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