Large-eddy Simulation of the Atmospheric and Ocean Boundary Layers and Implementation of Modelling on Computational Systems of Parallel Architecture

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Introduction

The processes which have place inside the atmospheric boundary layer (ABL) and ocean boundary layer (OBL) are similar to each other in many respects. It's known that along with small-scale isotropic turbulence the large-scale (compatible with the layers thickness) coherent motions are usually observed inside both ABL and OBL. These eddies can be induced by convection and by surface wind stress. They play significant role in momentum heat and moisture (salinity) transport near surface and thus in atmosphere-ocean interaction.

Deardorff (1973) suggested the large-eddy simulation (LES) approach which is based on the decomposition of the flow into large-scale and small-scale motions. The three-dimensional structure and the time evolution of large eddies are directly simulated, whilst the feedback effect of small eddies on the large-scale flow is parameterized. Now this approach is widespread for the modelling of ABL, but the LES models of BLO are still rare.

It seems to be attractive to compose the coupled LES model of two interactive boundary layers, as the large-scale eddies in ABL and OBL have the close spatial scales in some cases and are directly connected due to surface fluxes.

The number of grid points N in LES models are significantly less then in the case of direct modelling. It is found (Agee and Gluhovsky, 1999) that the 50-m grid simulation includes a significant portion of the inertial subrange, and therefore, for the domain $10 \times 10 \times 2.5$ km^3 the value of N is of order 10^6. Modern computers (even not parallel) allow to simulate successfully the ABL with such resolution. The same estimation of N takes place for the OBL LES model too, but here the size of domain is approximately 10-30 times less, since one needs to simulate OBL with the more precise grid to satisfy the demand of the resolution of some part of inertial subrange. The coupled modeling requires the same horizontal sizes for the both models. So the number of grid points in coupled model should be 10^2-10^3 times increased. Taking into account a number of prognostic variable (7 for each model in our case) and peculiarities of numerical scheme (multi-layer explicit schemes are often used) the total value of on-line storage in coupled ABL-OBL LES model can reach 10-100 Gigabytes.

It's clear that the single way to realize such model is using of the computers of parallel architecture, because we have the significant requirements both for storage and computer run time.

Here we present the short description of ABL and OBL LES models and some specialty of the parallel realization.

Models description

a. Basic equations

The LES models used in this work are based on equations of the Reynolds type. The set of governing equations is derived by a space averaging of the Navier-Stokes equations for in-

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compressible fluid expanded by the heat transport equation and moisture (salinity) transport equation. The systems of equations for ABL and OBL are almost identical except the state equations, which express the dependencies of the air and water densities on potential temperature, pressure and moisture and on temperature and salinity correspondingly. These equations are simplified, using the Boussinesq approximation, and are written in the tensor form as follows:

$$\frac{\partial \overline{u}_i}{\partial t} = -\frac{\partial}{\partial x_j}\overline{u}_i\overline{u}_j - \frac{\partial}{\partial x_j}\overline{u_i'u_j'} - \frac{1}{\rho_0}\frac{\partial \overline{p}}{\partial x_i} + \nu\frac{\partial^2 \overline{u}_i}{\partial x_j \partial x_j} + \frac{g}{\rho_0}\overline{\rho}\delta_{i3} - 2\varepsilon_{ijk}\Omega_j\overline{\mathrm{u}}_{\mathrm{k}}, \tag{1}$$

$$\frac{\partial \overline{\theta}}{\partial t} + \frac{\partial}{\partial x_j}\overline{u}_j\overline{\theta} = -\frac{\partial}{\partial x_j}\overline{u_j'\theta'} + \chi\Delta\overline{\theta}, \tag{2}$$

$$\frac{\partial \overline{s}}{\partial t} + \frac{\partial}{\partial x_j}\overline{u}_j\overline{s} = -\frac{\partial}{\partial x_j}\overline{u_j's'} + D\Delta\overline{s}, \tag{3}$$

$$\frac{\partial \overline{u}_i}{\partial x_i} = 0, \tag{4}$$

Using Reynolds equations (1) and equation of continuity (4) one can get Poisson equation for pressure:

$$\nabla^2\overline{p} = \rho_0\frac{\partial Q_i}{\partial x_i}, \tag{5}$$

were Q_i is the left side of (1) except the term including pressure p.
The nonlinear state equation (Bryden et al., 1999) was used for sea water:

$$\overline{\rho}_0 = \overline{\rho}_0\left(\overline{\theta}, \overline{s}, \overline{p}\right). \tag{6}$$

Correspondingly, the air density $\overline{\rho}_a$ is given by:

$$\overline{\rho}_a = \frac{\overline{p}}{RT_v}, \tag{7}$$

were $T_v = T(1+0,61q)$ - virtual temperature.

b. Subgrid closure

Equations (1), (2) and (3) contain the Reynolds subgrid stresses $\overline{u_i'u_{\mathrm{j}}'}$, subgrid heat flux $\overline{u_j'\theta'}$ and salinity moisture flux $\overline{u_j's'}$ which are responsible for the feedback effect of subgrid scales on resolvable motion. To parameterize these terms, the methodology proposed by Smagorinsky (1963) is used:

$$\overline{u_i'u_{\mathrm{j}}'} = -K_m\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \tag{8}$$

$$\overline{u_j'\theta'} = -K_h\frac{\partial \theta}{\partial x_i}, \tag{9}$$

$$\overline{u_j's'} = -K_h\frac{\partial s}{\partial x_i}, \tag{10}$$

where Km is the eddy viscosity and Kh is the eddy diffusivity. They are assumed to be functions of the subgrid turbulence kinetic energy $E = \overline{u_i'^2}/2$ and dissipation rate of turbulence kinetic energy $\in$ (the consequence of Kolmogorov hypothesis):

$$K_m = \frac{c_\mu E^2}{\in}. \tag{11}$$

Two additional prognostic equations for E and $\in$ are introduced (Monin and Yaglom, 1965):

$$\frac{\partial E}{\partial t}=-\frac{\partial \overline{u}_j E}{\partial x_j}+\frac{\partial}{\partial x_i}\frac{K_m}{\sigma_E}\frac{\partial E}{\partial x_j}+K_m\left(\frac{\partial \overline{u}_i}{\partial x_j}\right)^2-\delta_{i3}\frac{1}{\rho_0}K_h\frac{\partial \overline{\rho}}{\partial x_j}-\in, \qquad (12)$$

$$\frac{\partial \in}{\partial t}=-\frac{\partial \overline{u}_j E}{\partial x_j}+\frac{\partial}{\partial x_i}\frac{K_m}{\sigma_E}\frac{\partial \in}{\partial x_j}+c_1 S_\in / E+c_2 B_\in / E-c_3 \in^2 / e. \qquad (13)$$

Here B and S are buoyancy and shear production of TKE correspondingly.

The equations (12,13) should describe the turbulent motions with the subgrid spatial scales, so the dissipation rate of TKE is limited as follows:

$$\in > \in_{\min}=\frac{c_\in E^{3/2}}{l_{\max}}. \qquad (14)$$

Here the value of l_{max} is determined by the value of grid cells.

c. Boundary conditions

The calculations are performed in rectangular domains $[0 \le x \le L_x]$ x $[0 \le y \le L_y]$ x $[z_0 \le z \le L_z]$, where z_0 is the roughness length.

Horizontal boundary conditions are assumed to be periodic.

The vertical velocity ω at the bottom ($z = z_0$) and the top ($z = L_z$) are prescribed to be zero.

The momentum, heat and moisture (salinity) fluxes are set to zero at the top of ABL and the bottom of OBL.

The Monin-Obukhov similarity formulation (Monin and Yaglom, 1965) and Businger-Dyer empirical formulas (e.g., Sorbjan, 1989) are employed to calculate the momentum, heat and moisture fluxes near surface. This procedure is included only in ABL model. In OBL model the surface fluxes are prescribed by the constant values (in the case of modelling of OBL only) or are taken from ABL model in the case of coupled modelling.

d. Numerical scheme

A finite-difference approach is employed to perform numerical experiments. For the space approximation a full staggered grid with the uniform spacing is used. Partial differential equations of the model are approximated in space using a finite-difference technique with the second order of approximation. Matsuno scheme was used for the time approximation. The Poisson equation (5) is solved by multigrid method. Parallel code of this method written by Bernard Bunner was taken from http://www.mgnet.org

Parallel realization

Message Passing Interface (MPI) is used for the data exchange between processors. 3-D decomposition of area was applied. The most exchanges were based on nonblocking communications. The parallel version is oriented to supercomputers with shared memory. The codes of the models are written using the memory allocation faculties of Fortran 90. The on-line memory, used for the storing of prognostic variables of the models, is dynamically shared among the processors. So the memory restrictions are removed (in case of sufficient amount of processors). The testing of parallel model was carried out using cluster MVS-1000M of Joint Supercomputer Center.

The acceleration strongly depends on the ratio of numbers of boundary and inner points in the subdomains. For example if the total domain contains 96×96×32 grid cells the computer-run time of parallel version of LES model (32 processors in use) is in 15-16 times less than the run time of sequential code. This acceleration is not so big and grows slowly with increasing of number of processors. But on the other hand the acceleration of sequential version of the model with a small number of grid points wasn't the main goal of our work in this direction. The several numerical experiments were carried out with large domains. For example the parallel version of ABL LES model permits to use the domain containing 768 × 768 × 256 points (spatial resolution - 10 × 10 × 10 m^3). In this case we used 576 processors (decomposition - 12 × 12 × 4). Here the exchanges between processors take only 5-6% of run time. This experiment requires up to 15 Gigabytes on-line storage and a quite big run time, so it is unattainable with the help of sequential technique.

References

1. *E. Agee and A. Gluhovsky,* LES model sensitivities to domains, grids and large-eddy time-scales. *J. Atmos. Sci.*, 56 (1999), 599-604.
2. *J.A. Businger, J.C. Wyngaard, Y. Izumi, E.F. Bradley,* Flux-profile relationships in the atmospheric surface layer. *J. Atmos. Sci.*, 28 (1971), 181-189.
3. *J.W. Deardorff,* The use of subgrid transport equations in a three-dimensional model of atmospheric turbulence. *Journal of Fluids Engineering*, 9 (1973), 429-438.
4. *J. Smagorinsky,* General circulation experiments with the primitive equations: 1. The basic experiment. *Mon.Wea.Rev.*, 91 (1963), 99-164.
5. *Z. Sorbjan,* Structure of the atmospheric boundary layer. USA:Prentice-Hall,Inc.,1989,317 p.