PAPER • OPEN ACCESS

Numerical Prediction of Local Meteorological Processes above a City with a Supercomputer

To cite this article: A V Starchenko *et al* 2021 *J. Phys.: Conf. Ser.* **1740** 012071

Numerical Prediction of Local Meteorological Processes above a City with a Supercomputer

A V Starchenko, E A Danilkin, S A Prohanov, L I Kizhner and D V Lechshinsky

Tomsk State University, Tomsk, Russian Federation, 634050

E-mail: starch@math.tsu.ru, ugin@math.tsu.ru, sergey@prohanov.com, kdm@mail.tsu.ru, 360flip182@gmail.com

Abstract. This paper presents a parallel algorithm for numerical solution of equations for the non-hydrostatic mesoscale meteorological model TSUNM3. To justify the choice of the Message Passing Interface technology, computational experiments were performed to compare the effectiveness of the following parallelizing technologies: MPI, OpenMP, OpenACC, and CUDA. 2D decomposition of the gridded domain for the TSUNM3 model has been carried out with MPI technology. It allows for a numerical forecast for the next day in 17 minutes of CPU time on 144 cores of the TSU Cyberia computing cluster.

1. Introduction

Mathematical support for automated information systems of biosphere monitoring and warning about natural hazards, including atmospheric phenomena and adverse weather conditions that lead to a significant deterioration in atmospheric air quality and visibility, as well as for air traffic safety is a high priority issue in Hydrometeorology and related areas. Processes occurring in the atmospheric boundary layer have a significant impact on human life and activity. Fog, snowstorm, precipitation, glaze-ice and rime deposition, convective phenomena (thunderstorms, squall, tornado), and a number of other hazardous weather events have a significant impact on all sectors of economy, including land and air transport and power supply of industrial facilities. Moreover, dangerous weather events often result in catastrophic consequences.

Therefore, development of modern mathematical support and software for monitoring and early warning of dangerous meteorological conditions and conditions that lead to a significant deterioration in atmospheric air quality and visibility near large cities, industrial facilities and transport hubs is an urgent task.

The purpose of this work is to create a parallel version of the high-resolution non-hydrostatic mesoscale meteorological model TSUNM3 developed at Tomsk State University to predict dangerous weather events and atmospheric air quality over a city [1].

2. Mathematical Statement of the Problem and its Numerical Solution

2.1. Mesoscale meteorological model TSUNM3

The TSUNM3 mesoscale model (Tomsk State University Non-hydrostatic Mesoscale Meteorology Model) predicts wind speed components and temperature and humidity characteristics in the atmospheric boundary layer at 50 vertical levels (up to 10 km) for an area of 200x200 km with a nested domain of 50x50 km (grid step is 1 km). The model is initialized based on the results of the numerical forecast of the operational global numerical weather prediction model SL-AV of the Hydrometeorological Center of the Russian Federation [2]. The main features of the TSUNM3 model:

- non-hydrostatic approximation for motion equations and quasi-steady-state approximation for continuity equation [3];
- terrain following coordinate system with a variable vertical resolution;
- lateral boundary conditions of the "radiation" type (for horizontal velocity, temperature, and humidity components) [4], which take into account the spatial and temporal trends of dependent variables generated by the larger scale model (the SL-AV operational global model [2]);
- predictive model for soil temperature based on the heat equation and diagnostic ratio for moisture of the soil surface layer;
- surface heat fluxes calculated on the basis of Monin-Obukhov similarity theory;
- short-wave and long-wave radiation which takes into account the effects of cloud layer [5];
- the WSM6 [6] moisture microphysics considers generation of rain drops, clouds, snow, ice crystals, graupel from atmospheric moisture;
- prognostic equation for turbulence kinetic energy and algebraic relations for the scale of turbulence and turbulent diffusion [7].

The mathematical statement of the TSUNM3 model includes eleven non-stationary three-dimensional nonhomogeneous "convection-diffusion" equations (for the three components of speed, temperature, turbulence energy, moisture, raindrops, snowflakes, cloud moisture, ice crystals, graupel) and several closing algebraic relations where calculations are independent (can be performed simultaneously) in the vertical coordinate direction.

Let's review the generalized differential convection–diffusion equation:

$$\frac{\partial \rho\Phi}{\partial t}+\frac{\partial \rho u\Phi}{\partial x}+\frac{\partial \rho v\Phi}{\partial y}+\frac{\partial \rho w\Phi}{\partial z}=\frac{\partial}{\partial x}\left(K_{xy}\frac{\partial\Phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{xy}\frac{\partial\Phi}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z^{\Phi}\frac{\partial\Phi}{\partial z}\right)+S_{\Phi}, \quad (1)$$

where t,x,y,z are time and coordinates (axis Ox is directed to the East, Oy - to the North, Oz - upward vertically); u,v,w are velocity vector components; K_{xy},K_z^{Φ} turbulent transfer coefficients; S_{Φ} is the source term. Table 1 shows the values of Φ, K_z^{Φ} and S_{Φ} for each equation of the TSUNM3 model.

The equation of state is also added to the differential equations of the form (1):

$$p=\rho RT,\ \ R=R_0\left[\frac{1-q_V}{M_{air}}+\frac{q_V}{M_{H_2O}}\right]$$

Here p, T, q_V are pressure, temperature, and absolute humidity of the air; M, R_0 are molecular weight and the universal gas constant.

Newton's boundary conditions are used as the boundary conditions for (1) for the underlying surface, and Neumann boundary conditions for the upper boundary:

$$z=h(x,y):K_z\frac{\partial\Phi}{\partial z}=\alpha(\Phi-\Phi_0);\qquad z=H:K_z\frac{\partial\Phi}{\partial z}=\gamma_{\Phi} \quad (2)$$

Boundary conditions of the "radiation" type are used on the lateral boundary [4]:

$$x=-L;x=L:\frac{\partial\Phi}{\partial t}+C_{\Phi}^{x}\frac{\partial\Phi}{\partial x}=\frac{\partial\Phi_S}{\partial t}+C_{\Phi}^{x}\frac{\partial\Phi_S}{\partial x};\ y=-L;y=L:\frac{\partial\Phi}{\partial t}+C_{\Phi}^{y}\frac{\partial\Phi}{\partial y}=\frac{\partial\Phi_S}{\partial t}+C_{\Phi}^{y}\frac{\partial\Phi_S}{\partial y} \quad (3)$$

Here, "S" index corresponds to the parameters determined from the global scale model [2], but with a lower resolution; $C_{\Phi}^{x},C_{\Phi}^{y}$ are the phase velocities [4]. $2L$ is the horizontal size of the domain.

Journal of Physics: Conference Series **1740** (2021) 012071 doi:10.1088/1742-6596/1740/1/012071

Table 1. TSUNM3 mesoscale model equations

Equation	Φ	K_z^Φ	S_Φ	Equation	Φ	K_z^Φ	S_Φ
Continuity	1	0	0	Water moisture	q_V	K_z^h	ρR_V
u-momentum	u	K_z^m	$-\partial p/\partial x+\rho f v$	Rain water	q_R	0	ρR_R
v-momentum	v	K_z^m	$-\partial p/\partial y+\rho f u$	Cloud water	q_C	K_z^h	ρR_C
w-momentum	w	K_z^m	$-\partial p/\partial z-\rho g$	Snow	q_S	0	ρR_S
Energy balance	θ	K_z^h	$\theta\left(Q_{rad}-\rho L_w R_V\right)/c_p T$	Ice	q_I	0	ρR_I
Turbulence	k	K_z^m/σ_k	$P+G-\rho\varepsilon$	Graupel	q_G	0	ρR_G

Where θ is the potential temperature, k is the turbulence energy, q_R, q_C, q_S, q_I, q_G are the concentrations of raindrops, cloud moisture, snow, ice crystals, and hail in the atmosphere. P, G, ε are turbulence generation due to the wind shear, turbulence generation due to the buoyancy, and turbulence energy dissipation. Q_{rad} is atmosphere heating due to short-wave and long-wave radiation. L_w is the vapourization heat.

Initial conditions for the equation (1) are determined by the interpolation Φ_S computed on a coarser grid from the global scale model to a more detailed grid of the mesoscale meteorological model.

2.2. Numerical solution of the problem

The transformation of the following form is applied to equation (1) to take into account the inhomogeneous relief of the underlying terrain $h(x,y)$:

$$x'=x;\,y'=y;\,z'=\frac{z-h(x,y)}{H-h(x,y)}H \tag{4}$$

To solve the problem (1)-(3), structured grids are used with a uniform step in the horizontal directions of Ox and Oy and condensing grids to the Earth's surface in the vertical direction.

When approximating the differential formulation of the problem, we use the finite volume method with the second-order approximation in spatial variables and explicit-implicit approximations in time (Adams-Bashforth and Crank-Nicolson), which also provide second-order accuracy in time.

$$\Phi_h^{n+1}=\Phi_h^n+\frac{\Delta t_n}{2}\left(3L_h\left(\Phi_h^n\right)-L_h\left(\Phi_h^{n-1}\right)\right)+\frac{\Delta t_n}{2}\left(\Lambda_h\left(\Phi_h^{n+1}\right)+\Lambda_h\left(\Phi_h^n\right)\right)+\frac{\Delta t_n}{2}\left(3S_\Phi\left(\Phi_h^n\right)-S_\Phi\left(\Phi_h^{n-1}\right)\right) \tag{5}$$

Where $\Phi_h^n=\left\{\Phi_{i,j,k}^n\right\}$ is the grid function of the scalar Φ for which the differential equation (1) is given; L_h is the finite-volume analogue of the convective-diffusive operator in equations (1) except for the vertical diffusion along the axis Oz, Λ_h is the difference analogue of the differential operator of vertical diffusion $\frac{\partial}{\partial z}\left(K_z^\Phi\frac{\partial\Phi}{\partial z}\right)$, $S_\Phi(\Phi)$ is the source terms of equation (1). Implicit approximation for the vertical diffusion transfer, which is important in the boundary layer of the atmosphere, allows to avoid a more rigid restriction to the time integration step. When approximating the convective terms of equation (1), van Leer's monotonic linear upwind schemes are used [8]. Regular approximations of the second-order accuracy are applied for the diffusion terms. As a result of these approximations, a difference scheme is obtained to calculate the values of the grid function $\left\{\Phi_{i,j,k}^{n+1}\right\}$ where the tridiagonal matrix algorithm along the vertical grid lines can be used independently. Such method of difference scheme construction (5) gives it the property of linear dependence of the number of arithmetic operations on the size of the problem grid.

The "predictor-corrector" scheme is used to match the finite-difference values of the velocity and pressure vector field at each time step. Its main idea is that first, the grid values of the velocity vector components are predicted using difference schemes of the form (5) with the values of the pressure grid function p_h^n known on the *n*-th layer in time. Then, an elliptic difference equation is solved for the pressure correction $p'_h = p_h^{n+1} - p_h^n$ and the intermediate velocity and pressure fields are corrected. This operation is performed with the requirement that the corrected values of the velocity components shall satisfy exactly the difference analog of the continuity equation (1). Finite-difference equations for pressure correction p'_h are solved by Seidel's iterative line-by-line method [9] with red-black ordering of the computational grid nodes for each horizontal level k and implicit representation of the grid function values p'_h at nodes $(i,j,k+1)$, (i,j,k), $(i,j,k-1)$:

$$\begin{aligned} -ab_{i,j,k}\left(p'\right)^{l+1}_{i,j,k-1} + ap_{i,j,k}\left(p'\right)^{l+1}_{i,j,k} - at_{i,j,k}\left(p'\right)^{l+1}_{i,j,k+1} = ae_{i,j,k}\left(p'\right)^{l}_{i+1,j,k} + an_{i,j,k}\left(p'\right)^{l}_{i,j+1,k} + \\ + aw_{i,j,k}\left(p'\right)^{l}_{i-1,j,k} + as_{i,j,k}\left(p'\right)^{l}_{i,j-1,k} + b_{i,j,k}; \quad i=\overline{1,Nx};\, j=\overline{1,Ny};\, k=\overline{1,Nz}. \end{aligned} \tag{6}$$

l – iteration number.

3. Parallel algorithms for the numerical method of the TSUNM3 model

3.1. Parallel programming technology

To select a parallel programming technology for the numerical method of solving equations of the mesoscale meteorological model TSUNM3, computational experiments were previously carried out with the solution of one convective-diffusion equation of the form (1) using the following parallel programming technologies: OpenMP, MPI, OpenACC, and CUDA. Test computations were performed on a mesh of 256x256x32 nodes and 5000 time steps. The computations were performed on the TSU Cyberia cluster. One computation node of the cluster has the following characteristics: 48Gb RAM, 2xIntel® Xeon® X5670 (2.93 GHz). The average computation time of the sequential program on one computational node of the TSU Cyberia cluster is 1915.9 sec.

When using the Open Multi-Processing technology, the following parallelization method was chosen: the distribution of the general set of tasks of linear systems (5) solved by the tridiagonal matrix algorithm along the available threads of multicore processors. A speedup of 10.5 (182.5 seconds) was achieved on a single node of the Cyberia cluster with 12 cores with shared RAM. To implement the Message Passing Interface technology, the two-dimensional decomposition of the computational grid in horizontal Ox and Oy directions was performed using the Cartesian topology and message passing function: MPI_SendRecv. Fictitious cells were created along the perimeter of the subdomain to ensure the uniformity of the computations in each of the subdomains of the three-dimensional mesh. Finite-difference equations (5) were simultaneously solved in each subdomain along vertical grid lines by the tridiagonal matrix algorithm. With this method of parallel computations, one "convection-diffusion" equation (5) is solved in 16.3 seconds on 128 TSU Cyberia cluster cores (computation speedup is 117 times).

OpenACC and CUDA technologies were used to solve equation (1) on hybrid computing systems (CPU + GPU). When using OpenACC technology, the same way of arranging parallel computations was used as for OpenMP technology. The compiler directives were used to distribute the general set of linear equation tasks (5) along the available threads that implement computations on the GPU cores. The computation results with a parallel program created with the use of OpenACC technology on the NVidia RTX2080 Ti graphics card showed the runtime of about 20.4 seconds.

Parallelization with CUDA technology was based on the principle of two-dimensional (2D) data decomposition. The number of launched threads was 256 x 256, i.e. each parallel thread performed independent computations for the (i, j) -vertical grid lines. The compute kernel was executed for each time step with subsequent process synchronization. The CUDA parallel programming technology used to implement the algorithm under discussion allows obtaining problem solution in 16.6 seconds.

Thus, GPU-based computing is promising with a small amount of data transferred between software modules. However, if a program code contains several program modules with a large amount of information transferred between them during computations, the Message Passing Interface technology is advisable.

3.2. Parallel implementation of the numerical method for TSUNM3

Taking into account the results of the computational experiments presented above, the working version of the TSUNM3 model was parallelized using the MPI technology. Table 2 shows the obtained values of the speedup of the parallel program when performing computations for the local area of study on various grids during two days of simulation: 50x50x50 nodes (Grid 1) and 98x98x50 nodes (Grid 2).

The choice of grids for computations is determined by the size of the research area. In the first case, it is an area with a city with population of 1 million residents (the step size of the horizontal grid is 1 – 2km, the area is 50-100km), in the second case, it is an industrial district with a large number of enterprises with a large populated area in the center (the size of the research area is ~100-200km). For the selected grid sizes, the mesoscale model computations were carried out with the TSU Cyberia cluster.

Table 2. Parallel program speedup values for different grids and different numbers of processes

Processes	4	9	16	36	64	144
Grid 1	3.9	8.5	14.8	31.6	53.9	102.4
Grid 2	3.9.	8.7	15.3	33.0	57.9	121.5

Table 2 shows that the developed parallel algorithm demonstrates good scalability and high efficiency for a significant number of processes (up to 144). The obtained parallel program speedup results provide for forecasting calculations for the next day in 22 minutes of the program runtime on 144 cores of the cluster.

Besides, transition to single-precision computations in the TSUNM3 software was made to speed up the numerical prediction results. This reduced computer time to obtain a numerical daily forecast to 17 minutes on 144 cores. It should be noted that even with a smaller number of cores used in the calculation, the gain in the processor time of the calculation when switching to single-precision arithmetic is about 25%.

4. Conclusion

The two-dimensional latitude-longitude MPI decomposition of the grid domain with the chosen method to solve grid equations is the basis for an efficient parallel algorithm of solving TSUNM3 mathematical model equations with a good scaling degree. Computational experiments at the TSU Cyberia cluster have shown that the developed parallel algorithm provides for a numerical forecast of local weather conditions with a resolution of 1 km for the next day in 17 minutes of CPU time on 144 cores of the TSU Cyberia cluster.

Acknowledgments

The work was supported by the Russian Science Foundation (project no. 19-71-20042).

References

[1] Starchenko A V, Bart A A, Kizhner L I and Danilkin E A 2020 Mesoscale meteorological model TSUNM3 for the study and forecast of meteorological parameters of the atmospheric surface layer over a major population centerVestn. Tomsk. Gos. Univ. Mat. Mekh. **66** 35-55.

[2] Tolstykh M A, Fadeev R Yu, Shashkin V V, Goyman G S, Zaripov R B, Kiktev D B, Makhnorylova S V, Mizyak V G and Rogutov V S 2018 Multiscale Global Atmosphere Model SL-AV: the Results of Medium-range Weather Forecasts *Russ. Meteorol.Hydrol*. **43** 773–779.

[3] Nieuwstadt F T and Van Dop H 1984 *Atmospheric Turbulence and Air Pollution Modelling* (Dordrecht, Holland: Springer) p 358

[4] Carpenter K 1982 Note on the Paper «Radiation Condition for the Lateral Boundaries of Limited-Area Numerical Models» by Miller M. and Thorpe A. (Vol. 107. pp. 615–628) *Journal of Royal Meteorology Society* **108** 717-719.

[5] Avissar R and Mahrer Y 1988 Mapping Frost-Sensitive Areas with a Three-Dimensional Local-Scale Numerical Model. Part I. Physical and Numerical Aspects *Journal of Applied Meteorology* **27** 400-413.

[6] Hong S.-Y and Lim J.-O J 2006 The WRF single-moment 6-class microphysics scheme (WSM6) *J. of Korean meteorological society* **42**(2), 129-151.

[7] Belikov D A and Starchenko A V 2007 Numerical model of turbulent pollutant transport in the atmospheric boundary layer *Atmospheric and oceanic optics* **20**(8) 607-612.

[8] Van Leer B 1974 Towards the ultimate conervative difference scheme: II. Monotonicity and conservation combined in a second order scheme *Journal of Computational Physics* **14** 361-370.

[9] Danilkin E A and Starchenko A V 2010 High Performance Computation for Large Eddy Simulation *LNCS series* **6083** 163-172.