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A parallel algorithm for solving the mantle flows non-stationary problem*

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Abstract. A parallel version of the program for the simulation of flows in the Earth's mantle has been developed. A non-stationary model of the mantle flows describes a compressible medium with strongly varying rheological and transport properties. It is based on the solution of the Navier–Stokes equations. The numerical model includes both explicit and implicit finite difference schemes implemented by vector fitting. The parallel algorithm has been analyzed in detail. The parallel algorithm provides nearly linear acceleration, despite the use of vector fitting. The main characteristics of the parallel algorithm are presented. The total time computation and the inner loop for a given accuracy of calculation varying for different sizes of grid spaces have obtained. The inner loop is used to compute the mantle flow velocities along the coordinate computing space. The dependence of speedup and efficiency on the size of the grid computing space is shown. A weak dependence of these parameters on a specified accuracy of the calculations is shown. The description of the process of melting and diapirism in the lower crust is obtained by calculations on a multiprocessor system. The structure of the floating granite magma has been determined.

Introduction

Geodynamics is the study of the nature of the underlying forces and processes that occur as a result of the Earth's planetary evolution. The evolution of gravitational unstable systems in the Earth is one of the currently central problems of geodynamics. The solution to this problem is connected with the analysis of the processes of heat and mass transfer in the Earth's crust. The problem of stability or redistribution of matter and energy in the Earth's interior is currently being studied within the equilibrium thermodynamics and non-isothermal continuum mechanics. One possible fruitful approach is to consider the material of the Earth's crust as a continuous medium. Then, in the study of deformation in geological time, the conservation laws for the elastic-plastic / viscous material can be used with some restrictions. Among the endogenous mechanisms for the transport of matter in the Earth's crust and in the upper mantle, the movement caused by the gravitational instability and heat fluxes plays a decisive role.

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The formation of large igneous provinces in the continental and in the oceanic plates are associated with the lower mantle super-plumes rising from depths of the interface of the mantle and the core [1]. The physical aspects of the floating plume of thermal or thermal-chemical nature have been thoroughly investigated with physical and mathematical modeling [2, 3]. This concept includes floating in a local region of a light, high-temperature and low-viscous mantle material (plume) on the background of large-scale convective flows. Obscure questions remain about the final stage of the evolution of diapirs, namely, how high they can climb. What is the ratio of the lift and the drag of a viscous substance when rising to the upper levels of the lithosphere. Thus, the mechanism of transporting the magma diapir in the most viscous and cold part of the mantle lithosphere requires a detailed study.

Geodynamics exploits the data of geology, geochemistry and geophysics, as well as data of mathematical and physical modeling of the underlying processes. Mathematical modeling is of great concern in geodynamics, allowing the check of the bright ideas and making fundamental discoveries. The development of mathematical modeling due to the progress of computing technology, which allows one to take into account the ever increasing set of interrelated physical processes in a wide range of scales. However, a powerful computer technology is only one of the needs of the numerical simulation. Another, a much more important requirement is the availability of suitable numerical algorithms and codes to be capable of efficient operations on available computers to study the physical problems of interest with a good accuracy and the most flexible approach to the introduction of the new physical processes. The simulation of the mantle flows has some specific features. Therefore, not all well-established methods are applicable to this type of problems. The current level of modeling involves multidimensional and high-resolution models. This brings about the need in a multi-processor computing technology. Expansion of models leads to the new requirements for the methods used for solutions. This contributes to their further development. In contrast to the conventional approach, based on the Boussinesq approximation, the model in question is based on solving a system of complete classical Navier–Stokes equations. They describe the dynamics of a weakly compressible flow with variable density and viscosity. Nonlinear equations of the model make necessary to use methods of solutions based on the computer-aided technologies. A parallel version of the algorithm is designed to obtain more accurate solutions. It is implement in Supercomputing Center Information Technology Center (ITC) NSU (www.nusc.ru). The computer system with shared memory is selected with allowance for a specific features of a numerical model, characterized by a large number of vector-runs and does not require more than a dozen processors for parallelization.

1. Mathematical model

Historically, the first and simple model of the mantle convection is a classical model of a viscous incompressible fluid based on the Stokes equations system [4]. Further, an approximate system of equations describing the convection of fluids and gases (called the Boussinesq approximation) was formulated. This model is wide spread in the numerical modeling of geodynamic processes, the convective currents environment [5–8]. A comprehensive analysis of methods for the numerical integration of the Stokes and the Boussinesq equations is found in [9,10]. To calculate the steady flows, more efficient seems to use methods based on the introduction of an artificial compressibility [11]. An example of the successful use of this approach to the simulation of the essential three-dimensional processes in the Earth's mantle is given in [12]. In the Boussinesq approximation, the density changes in the flow are partially taken into account. In this case, density is dependent only on the temperature when determining the mass force. The refusal from some assumptions does not affect the basis of a viscous incompressible fluid, such as the constancy of thermal and transport properties of the gas, assumptions about a negligible role of the processes of dissipation of mechanical energy of a flow and pressure forces. Obviously, a modification of the model of an incompressible fluid cannot be used to describe flows with a significantly varying density due to the use of the incompressibility equations.

Let us consider a system of equations that describes the dynamics of a viscous liquid that is closed by the equation of state:

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \vec{u}) = 0,$$

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u}\nabla)\vec{u} = -\frac{1}{\rho}\nabla p + \frac{1}{\rho}\frac{\partial}{\partial x_k}\eta\Big(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} - \frac{2}{3}\delta_{ik}\frac{\partial u_m}{\partial x_m}\Big) + ge_y,$$

$$\frac{\partial T}{\partial t} + (\vec{u}\nabla)T = \nabla k \nabla \cdot T.$$

The equation of state is a direct result of the expression for the density $\rho = \rho_0(1 - \alpha T + \beta(p - p_0))$:

$$p = p|_{y=0} + \frac{1}{\beta}\Big(\frac{\rho}{\rho|_{y=0}} + \alpha T - 1\Big),$$

where ρ is the density, $\vec{u} = (u_x, u_y)$ is the velocity vector, T is the temperature, and p is the pressure, η is the viscosity, g is the acceleration of free fall, k is the thermal diffusivity, $\rho_{t=0}$ and $p_{t=0}$ are the density and the pressure at the initial moment of time, respectively.

Characteristic values of the variable are: $L_0 = 3 \cdot 10^4$ m, $\rho_0 = 2.8 \cdot 10^3$ kg/m^3, $T_0 = 550\,^\circ$C, $p_0 = \eta_0 k_0 / L_0^2$ Pa, $k = 10^{-6}$ m^2/s, $t_0 = L_0/k$, $u_0 = L_0/t_0$. The parameters $\alpha = 3 \cdot 10^{-5}$ 1/°C, $\beta = 10^{-11}$ 1/Pa are used in

the equation of state. To determine the viscosity of the model the Arrhenius equation is employed: $\eta = A \cdot \exp\left(\frac{E}{RnT}\right)$, where $A = 1.2 \cdot 10^{17}$, $E = 2.16 \cdot 10^4$, $n = 2.6$ are experimental data, R is a universal gas constant. In the given statement of the problem, the values of the viscosity coefficient are within the interval $\eta = 10^{18} \div 10^{20}$ Pa/s, therefore, $\mathrm{Pr} = \frac{\eta_0}{\rho_0 k_0} = 3.6 \cdot 10^{20} \div 3.6 \cdot 10^{22}$, $\mathrm{Ra} = \frac{\alpha g \rho_0 \theta L_0^3}{\eta_0 k_0} = 2.7 \cdot 10^2 \div 2.7 \cdot 10^4$, where θ is a characteristic temperature difference. In this model, the normal crust with exponential distribution of radioactive sources of heat is considered.

Choosing a model of a weakly compressible liquid is defined as desire to use a more complete model of the process with the density jumps caused by the melting phase transitions, and the ability to create a numerical technology of solution employing well-tested finite difference schemes. The criterion of applicability of the classical Oberbeck–Boussinesq model [13] to describe the thermal gravitational convection is known. If the parameter $\xi = \frac{g L_0^2 \rho_0}{\eta_0 k_0}$ is of order of less than or equal to one, the Oberbeck–Boussinesq model is not applicable. The value of ξ characterizes a relative contribution of the buoyancy factors and volume expansion of a fluid when forming the velocity field. In this class of problems the viscosity coefficient can vary in the limit $\eta = 10^{14} \div 10^{28}$ Pa/s, the parameter ξ being from 10^5 and 10^{-9}.

It is well known that the numerical integration of the full Navier–Stokes equations is a very complex and time-consuming computing task. It requires the development of special finite difference schemes and numerical algorithms. A significant difference of the mantle convection problems is the Prandtl numbers of order 10^{20}, the nonlinear equation of state, different scales of various processes strongly (by tens orders of magnitude) varying viscosities. These features create additional difficulties in the numerical implementation of the model taking into account the compressibility of a medium. However, it is now possible to carry out the numerical simulation of the most detailed models of the convection currents in view of strongly varying rheological and transport properties such as viscosity, density and thermal conductivity.

2. A parallel algorithm

In the case of low characteristic speeds of geodynamic processes (a few centimeters per million years) such problems are characterized by a high speed of sound and a small Mach number: $c = \sqrt{\frac{\partial p}{\partial \rho}} = \sqrt{\frac{1}{\beta \rho_0}} = 10^4$ m/s, $M = \frac{v_0}{c} = 10^{-13}$.

Geodynamics examines very slow flows, therefore in theory the Mach number, in contrast to other parts of seismology and geophysics, was not

used. The Mach number that was formally evaluated, one can refer to the experience in the field of computing significantly subsonic flows. It is known [14] that a decrease in the characteristic Mach number of the flow below 0.1 causes slowing down the convergence of iterations with respect to time in the method of determination and deterioration of the accuracy of the solution obtained.

The slowdown of the convergence of the method of determination is explained by the stiffness (increasing for $M \to 0$) of the dynamics equations of a compressible gas, defined as the ratio of a maximum and a minimum eigenvalues of the Jacobi matrix of convective flows vectors. A detailed study of this effect with the use of difference schemes, grid and flow parameters was carried out in [15]. In order to overcome problems with convergence, the method of preconditioning was proposed [14,16]. At the same time, Sagittarius and Shur [17] successfully applied the "compressibility scaling method" to calculate the viscous compressible gas flows for $M \ll 1$. A similar approach was proposed for the numerical simulation of flows and heat transfer in liquids with parameters close to the thermodynamic critical point [18]. Thus, the approaches similar to the method of preconditioning, but adapted to this class of problems are widely used.

To scale the elements of solving the system of equations, the equations are reduced to a dimensionless form with dimensionless parameters of the current $\hat{K} = \frac{k_0\eta_0}{\alpha\rho_0\theta}$, $\hat{\beta} = \frac{\beta k_0\eta_0}{L_0^2}$, $\hat{\alpha} = \alpha T_0$, $\hat{p} = p|_{y=0}/p_0$, $\hat{\rho} = \rho|_{y=0}/\rho_0$ [19]. All the parameters of the flow are presented in the form of $f = f_0 f'$, where f' is a physical characteristic, f_0, f' are its characteristic and dimensionless values, respectively. To solve the problem, we introduce non-stationary fictitious time iterations [20] for the equations of motion. Following the ideology of the considered approaches let us multiply the fictitious time derivative by a factor k_{pr} having the value of order of the Prandtl number. At each real-time step, iterations for the equations of motion are performed with respect to fictitious time. The modified equations will not be stiff thus ensuring the convergence to a desired solution at each at real-time step. The resulting system of equations in dimensionless variables has the form:

$$\frac{\partial\rho}{\partial t} + u_x\frac{\partial\rho}{\partial x} + u_y\frac{\partial\rho}{\partial y} + \rho\Big(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y}\Big) = 0,$$

$$k_{\rm pr}\frac{\partial u_x}{\partial\tau} + \frac{\partial u_x}{\partial t} + u_x\frac{\partial u_x}{\partial x} + u_y\frac{\partial u_x}{\partial y} = \mathrm{Pr}\frac{1}{\rho}\Big(-\frac{\partial p}{\partial x} + \frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y}\Big),$$

$$k_{\rm pr}\frac{\partial u_y}{\partial\tau} + \frac{\partial u_y}{\partial t} + u_x\frac{\partial u_y}{\partial x} + u_y\frac{\partial u_y}{\partial y} = \mathrm{Pr}\frac{1}{\rho}\Big(-\frac{\partial p}{\partial y} + \frac{\partial\sigma_{xy}}{\partial x} + \frac{\partial\sigma_{yy}}{\partial y}\Big) + \mathrm{Ra}\,\hat{K},$$

$$\frac{\partial T}{\partial t} + u_x\frac{\partial T}{\partial x} + u_y\frac{\partial T}{\partial y} = \frac{\partial}{\partial x}k\frac{\partial T}{\partial x} + \frac{\partial}{\partial}k\frac{\partial T}{\partial y},$$

where

$$p = \hat{p} + \frac{1}{\hat{\beta}}\Big(\frac{\rho}{\hat{\rho}} + \hat{\alpha}T - 1\Big),$$

and the tensor of viscous stresses is

$$\sigma_{xx} = \eta\Big(\frac{4}{3}\frac{\partial u_x}{\partial x} - \frac{2}{3}\frac{\partial u_y}{\partial y}\Big), \quad \sigma_{yy} = \eta\Big(\frac{4}{3}\frac{\partial u_y}{\partial y} - \frac{2}{3}\frac{\partial u_x}{\partial x}\Big), \quad \sigma_{xy} = \eta\Big(\frac{\partial u_x}{\partial y} - \frac{\partial u_y}{\partial x}\Big).$$

Numerical integration of the full Naiver-Stokes is an extremely complex and time-consuming task. The peculiarity of the numerical implementation of the full Naiver-Stokes equations for flows with small Mach numbers is in a significant difference between the two characteristic significantly subsonic time scales: the characteristic time of the convection processes $t = L/v$ and the characteristic time of the acoustic perturbation $\tau = L/(vc)$. When using explicit finite difference schemes (according to the Courant stability condition) the time step can not exceed the characteristic time of the most rapid process of transmission of acoustic disturbances. Therefore, the use of explicit finite difference schemes is completely unjustified, except for certain specific tasks. The numerical model is implemented on a regular rectangular grid in the Cartesian coordinate system. The system of equations of motion (the inner cycle) is implemented by an implicit finite difference method of stabilizing corrections of first order with respect to time and space. In the inner cycle iterations are carried out with a fictitious time to ensure the accuracy of ϵ. An explicit upwind scheme is used for the implementation of the continuity equation and temperature in the outer cycle with a real time. The system of equations is solved for the deviation from the hydrostatic pressure, the initial density distribution being defined by the Runge–Kutta 4th order accuracy.

A parallel algorithm of the problem in question is implemented on the computer system with shared memory (IVC NSU). The algorithm is implemented in Fortran using the parallelization algorithms software in the general field of OpenMP memory. The computational domain is defined by a rectangle in the plane (X, Y). In the computational domain, a uniform rectangular grid of (iDimX, iDimY) size is given. The values of each parameter of the problem are identified in the grid. They are stored in 15 arrays of (iDimX, iDimY) size. The flow parameters: density, temperature and pressure are calculated by explicit schemes of the through calculation (without distinguishing features) on a 5-point pattern “cross”. Speeds along the coordinates are calculated by implicit schemes on a 5-point pattern “cross”.

Parallelization of the algorithm is in extracting parts (subdomains) of the computational domain and the distribution of these sub-regions by threads. The subregion distributed computation for each thread is assigned to it in sub-domains. The computational domain is conditionally “cut” into strips along either the coordinates X or Y. They are statically allocated by means

of OpenMP threads for calculations with this program. Note that points of the adjacent bands, which are necessary to calculate the pattern "cross", are available to all threads, since all the data are in the shared memory. The flow parameters: density, temperature, pressure are calculated by explicit schemes with splitting along the spatial directions [21]. These strips are calculated along one of the coordinates. The speed parameters are calculated in the inner loop of the program by an implicit scheme by the sweep method. Their calculation is carried out along both coordinates. Arrays to store the marching factors are set in the local memory of each thread, thus allowing carrying out the reverse flow passage (in the sweep algorithm) for each row or column of the strip calculated by them.

3. Acceleration and efficiency

In the development of a parallel algorithm it is important to know the potential of accelerating calculations and overheads associated with organization of parallelization of flows, their interaction and synchronization. In addition, it is important to know the performance metrics of a parallel algorithm on a computer system that allows one to compare it with other parallel algorithms. Also, it is needed to evaluate the possibility of parallel implementation on computer systems with shared memory with a large number of processor cores.

The computing node cluster of the ITC NSU is used as a computing system with a common field of memory for the numerical implementation of the algorithm. The computing nodes of the cluster consist of two 4-core Intel Xeon processors 5355, running at 2.66 GHz and 16 GB of the total RAM.

Figure 1 presents graphs of the computation of the total time as well as of the inner loop associated with computing speeds. The graphs are given for the size of a net space of 5,000 × 1,000 for the two values of accuracy $\varepsilon = 10^{-3}$ and $\varepsilon = 10^{-4}$. The graphs show the following. First, that a high precision of calculations considerably increases the computation time. Second, the time of computing the inner loop takes a considerable share of the total calculation time. On one and on eight threads, the total time of calculation, depending on the values of ε increases, approximately, 3.3 times.

Figure 2 presents graphs of the total calculation time for the two sizes of the grid spaces 5,000 × 1,000 and 10,000 × 2,000 with the accuracy of calculation $\varepsilon = 10^{-3}$. The graphs show that the dimensions of space considerably increase the time of calculation: on one thread in 5.4 times, and on eight threads in 9.4 times.

The acceleration factor U_p on R threads is calculated as: $U_p = \frac{T_1}{T_p}$, where T_1 is the time of calculating the problem on a single thread, T_p is the time of calculating the problem on P threads. Figure 3 presents graphs

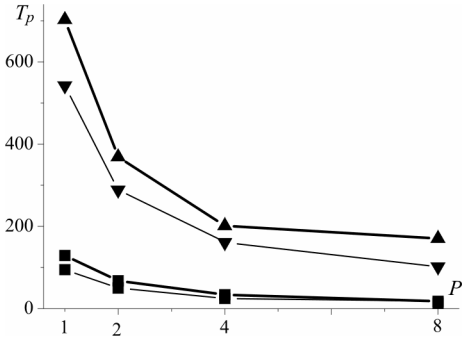

Figure 1. The total time of computation (triangles) and the time needed for computing the inner cycle (squares) when $\varepsilon = 10^{-3}$ and 10^{-4} for 2, 4, and 8 streams

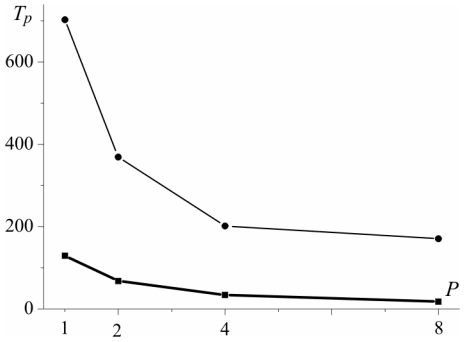

Figure 2. The total time of computation for 5,000 × 1,000 grid spaces (circles) and 10,000 × 2,000 (squares) when $\varepsilon = 10^{-3}$

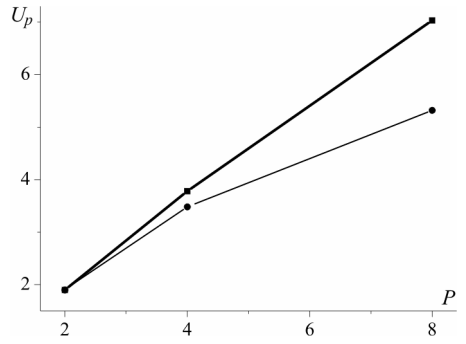

Figure 3. Acceleration of computation for 5,000×1,000 grid spaces (circles) and 10,000 × 2,000 (squares) for 2, 4, and 8 threads

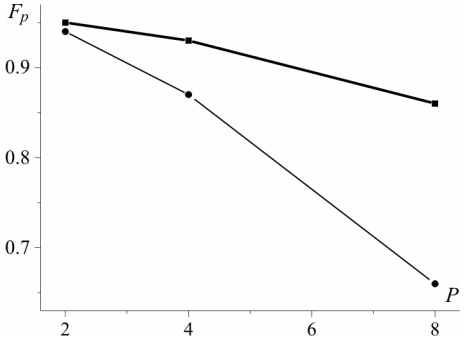

Figure 4. Efficiency of computation for 5,000 × 1,000 grid spaces (circles) and 10,000 × 2,000 (squares) for 2, 4, and 8 threads

of the calculation acceleration for 2, 4 and 8 threads for different sizes of grid computing space, specified by the number of grid points along the coordinates calculated with with the accuracy of $\varepsilon = 10^{-3}$. For $\varepsilon = 10^{-4}$, the graphs differ only slightly from those shown above, hence the accuracy of calculating the speed ε has a little effect on the acceleration rate. The graphs show that the size of the grid space has a significant effect on the acceleration of a parallel algorithm towards its reduction with increasing the size of the grid space.

The efficiency ratio F_p on P threads is calculated as: $F_p = \dfrac{T_{pc}}{T_{pc} + T_{ps}}$, where T_{pc} is the time of "pure" calculation of the problem (excluding any other costs) on P threads, T_{ps} is the total time spent on interaction and synchronization of P threads. The calculations were performed on the same

thread as the calculation of a sequential program. In the script of the program run it is indicated that the calculations are carried out on a unit only by a single thread. In all the cases, the program was invoked exclusively on a unit (exclusively means that resources on a unit are given exclusively to the program). This is due to the prevention of interference from other user tasks or from other cores of this unit that are not calculated at a given moment. This provides a greater accuracy of testing.

Figure 4 shows the effectiveness of the algorithm calculated with the accuracy of $\varepsilon = 10^{-3}$. For $\varepsilon = 10^{-4}$ the graphs differ only slightly from those presented above. The graphs show that the size of the grid space similar to acceleration has a significant influence on the performance of a parallel algorithm, its size decreasing with increasing the number of computational grid nodes.

4. Solution of the model problem

The objective of this paper is to construct a numerical model to describe the gravitational unstable processes in the lithospheric mantle of the ancient cratons. The gravitational instability is considered to be a result of melting of the base of the lithosphere by heating its area of the anomalous mantle. Based on the model developed we will judge of the main regularities of the mantle diapirism of the basic or ultrabasic magma. Magma rises through the "cold" high-viscosity lithosphere. The considered model [22] is based on geological, petrological and geophysical data, characterizing the structure and composition of the Siberian platform. The geometry of the model describes the structure of the lithosphere of the Siberian craton: 45-km-long crust and 155-km mantle lithosphere are considered. The total thickness of the lithosphere is 200 km, its value is assumed to be constant. The rectangular area of the Earth's crust 200 km in depth and 1000 km in width is considered. The free surface with a constant value of zero temperature, the density $2.8 \cdot 10^3$ kg/m and pressure 10^5 Pa are set at the upper boundary of the area. The lateral boundaries of the area are isolated for the heat transfer and for the release of a substance. The area of 100 km in width is set at the lower boundary. This area is constantly heated up to the temperature of 1450 °C, i.e., the process of "underplating" is considered. On the rest of part the lower boundary the temperature of 1350 °C is set.

A cycle consisting of the diapir rise to a maximum height of the pour point and at the termination of the heat source, or the establishment of a steady-state convection with a constant action of the heat source, has been simulated in [23].

Thus, the size of the grid space has a major influence on the speedup and efficiency of the parallel algorithm of the problem, while the calculation accuracy of the rate ε has a very weak effect. A detailed analysis of the

parallel algorithm has shown that it is possible to obtain the speedup to be close to linear for the grid spaces of a medium size, about $(5{,}000 \times 1{,}000)$ in spite of using the vector factorization.

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