Numerical Simulation of Three-Dimensional Viscous Flows with Gravitational and Thermal Effects


* International Institute of Earthquake Prediction Theory and Mathematical Geophysics, Russian Academy of Sciences, Varshavskoe sh. 79, korpus 2, Moscow, 113556 Russia
** Institute of Mathematics and Mechanics, Ural Division, Russian Academy of Sciences, ul. S. Kovalevskoi 16, Yekaterinburg, 620219 Russia

Received August 9, 2000

Abstract—A three-dimensional model of slow thermal convection in a highly viscous fluid with temperature-dependent density and viscosity is considered. The model is described by the equations of quasi-steady viscous inhomogeneous incompressible flow, transport equations for density and viscosity, and a heat balance equation. The numerical solution is based on the introduction of a vector velocity potential and on the application of a finite element method with a tricubic-spline basis for computing the potential. The transport equations were solved by the method of characteristics. The heat equation was solved by a finite-difference method based on a tridiagonal algorithm. A new two-component representation (in some cases, a one-component representation) was found for the velocity potential, which made it possible to substantially reduce computational costs. The numerical algorithms employed were designed to be implemented on parallel computers. The principal results of the study are summarized as follows: a numerical method is developed for simultaneous solution of the Stokes flow equation, heat balance equation, and transport equations for physical parameters of the fluid; it is demonstrated that computational costs can be reduced by reducing the dimensionality of the vector velocity potential; a characteristic example is computed.

INTRODUCTION

We consider the numerical simulation of three-dimensional, inhomogeneous, highly viscous, incompressible flows involving gravitational and thermal effects. Problems of this kind frequently arise in geophysics when various processes taking place in the earth’s interior are to be modeled [1–4]. A particular problem of interest is the simulation of evolution of argillaceous and saline formations in the crust, development of sedimentary basins, thermally driven convection in the earth’s mantle, and other processes. Three-dimensional numerical models of geophysical processes provide a basis for the most realistic simulations, but entail high computational complexity, which can be dealt with only on high-performance computers. Therefore, solution of three-dimensional problems must rely on highly efficient computational methods. Moreover, their numerical implementation frequently requires special procedures consistent with the architecture of the computer employed.

In geophysical problems, three-dimensional simulations of thermally driven convection in a rectangular domain have been performed by various investigators both for constant viscosity (e.g., see [5–7]) and for variable viscosity (e.g., in [4, 8–13]). They were based on the use of finite-difference, spectral, and multigrid methods.

In this paper, we propose methods and algorithms that can be used in numerical simulations of the problems mentioned above on modern parallel computers. The numerical simulation of the problem analyzed here relies on general equations of inhomogeneous, viscous, incompressible flow: a momentum equation, a heat balance equation, transport equations for physical parameters of the fluid, and an equation of state. These equations are modified and simplified by taking into account certain fluid properties and flow characteristics (high viscosity and low velocity). We eliminate the convective terms from the equation of motion (since the Reynolds numbers of typical flows under study are very low) to reduce it to the corresponding Stokes quasi-steady flow equation. We introduce a vector velocity potential and transform the governing equations, applying the curl operator to eliminate the incompressibility condition and pressure. The vector velocity potential is approximated by a linear combination of suitable basis functions consisting of certain localized tricubic splines. The approximation is determined from an appropriate variational equation corre-
Corresponding to the Stokes flow equation. We write out a system of linear algebraic equations for the approximation coefficients, which has a high dimension even for relatively coarse grid discretizations of the computational domain. This system is nonsingular by virtue of a special choice of basis functions in the finite element method, but the condition number of its matrix tends to infinity as the computational grid is condensed. Such systems of equations must be solved repeatedly, because their coefficients and right-hand sides are updated at each time step. This leads to certain conditions to be satisfied by the choice of solution procedures, and parallel algorithms prove to be definitely advantageous, since test computations have shown that a greater part of the CPU time resources consumed is required to solve the systems of equations in question. Density and viscosity are found by solving the corresponding first-order partial differential transport equations or the ordinary differential equations for the characteristics of the transport equations (with subsequent transfer of the initial density and viscosity along the characteristics). Temperature is determined from the heat balance equation by a finite-difference method. The well-posedness and solvability of the corresponding two-dimensional boundary value problems were analyzed in [14, 15].

Numerical analysis of problems of this type is difficult to perform because of the high dimensionality of finite-difference approximations. Considerable progress achieved in dealing with this difficulty became possible by making a special set of basis functions in the finite element method and using a two-component representation of the vector velocity potential proposed here. As a consequence, we managed to reduce computational costs and obtain adequate qualitative and quantitative results for relatively low-dimensional discretizations.

In what follows, we state the problem, restate it in a more tractable form, describe the overall computational procedure and some of its details, and present the results obtained by computing a model example reflecting some essential features of the real process.

1. DESCRIPTION OF THE MODEL AND STATEMENT OF THE PROBLEM

In a spatial domain $\Omega$, consider an inhomogeneous viscous incompressible flow in the presence of a gravity field and a temperature gradient. We describe the flow in terms of Eulerian variables. In Cartesian coordinates, the flow is governed by the following well-known equations [16–19]:

- the momentum (Navier–Stokes) equations
  \[
  \rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u}\right) = -\nabla p + \text{div}(\mu \mathbf{e}) + \mathbf{F},
  \]

- the incompressibility condition
  \[
  \text{div} \mathbf{u} = 0,
  \]

- the heat balance equation
  \[
  \frac{\partial}{\partial t}(\rho c T) + (\mathbf{u} \cdot \nabla (\rho c T)) = \text{div}(k \nabla T) + \mu \Phi + \rho Q,
  \]

- the equation of state for density
  \[
  \rho(t, x) = \rho_\infty(t, x)\left[1 - \alpha(T(t, x) - T_0)\right],
  \]

- the rheological equation for viscosity
  \[
  \mu(t, x) = \mu_\infty(t, x)\exp\left(\frac{E + \rho_\infty g x_3 V}{RT} - \frac{E_0 + \rho_\infty g x_3 V}{RT_0}\right),
  \]

- and the transport equations for thermally unperturbed density and viscosity
  \[
  \frac{\partial \rho_\infty}{\partial t} + (\nabla \rho_\infty \cdot \mathbf{u}) = 0, \quad \frac{\partial \mu_\infty}{\partial t} + (\nabla \mu_\infty \cdot \mathbf{u}) = 0.
  \]

Equations (1)–(6) contain the following variables and parameters: time $t$; a spatial point $x$ with Cartesian coordinates $(x_1, x_2, x_3)$; flow velocity vector $\mathbf{u} = (u_1(t, x), u_2(t, x), u_3(t, x))$; pressure $p = p(t, x)$; absolute temperature $T = T(t, x)$; density $\rho = \rho(t, x)$; viscosity $\mu = \mu(t, x)$; thermally unperturbed density $\rho_\infty = \rho_\infty(t, x)$; thermally unperturbed viscosity $\mu_\infty = \mu_\infty(t, x)$; gravitational acceleration $g$; universal gas constant $R$; external body force (gravity) per unit volume $\mathbf{F} = -g\mathbf{e}_3 = (0, 0, -g)$; unit basis vector $\mathbf{e}_3$ for the $Ox_3$ axis; specific heat $c$; heat conductivity $k$; coefficient of thermal expansion $\alpha$; activation energy $E$; activation volume $V$; a
dissipation function $\Phi = \Phi(t, x)$ representing the rate of heat production due to internal friction; the rate of heat production per unit volume due to nonviscous heat sources $Q = Q(t, x)$; and reference physical parameters $\rho_0$, $g_0$, $l_0$, $E_0$, $V_0$, and $T_0$ defined below.

Here, $\nabla$, div, and $e_{ij}$ denote the gradient operator, the divergence operator, and the rate-of-strain tensor $(e_{ij} = e_{ij}(u) = du_i/dx_j + du_j/dx_i)$, respectively:

$$\text{div}(\mu e_{ij}) = \left(\frac{3}{m = 1} \sum \frac{\partial (\mu e_{m1})}{\partial x_m}, \frac{3}{m = 1} \sum \frac{\partial (\mu e_{m2})}{\partial x_m}, \frac{3}{m = 1} \sum \frac{\partial (\mu e_{m3})}{\partial x_m}\right),$$

$$\Phi = \frac{1}{2} \sum e_{ij}^2.$$

Equations (1)–(6) make up a closed set of equations that determine the unknown $u_1$, $u_2$, $u_3$, $T$, $p$, $\rho$, and $\mu$ as functions of independent variables $t$ and $x$. Appropriate initial and boundary conditions for the desired functions are formulated below.

Thus, we seek functions $u_1 = u_1(t, x)$, $u_2 = u_2(t, x)$, $u_3 = u_3(t, x)$, $T = T(t, x)$, $p = p(t, x)$, $\rho = \rho(t, x)$, and $\mu = \mu(t, x)$ that satisfy both Eqs. (1)–(6) in a domain $\Omega$ at $t \geq t_0$, where $t_0$ is an initial moment, and prescribed boundary and initial conditions.

2. TRANSFORMATION OF THE PROBLEM

Equations (1)–(6) can be simplified by changing to dimensionless quantities and taking into account the characteristic values of these quantities. As characteristic values of parameters and variables, we introduce the following reference quantities: length $l_0$, density $\rho_0$, viscosity $\mu_0$, temperature $T_0$, specific heat $c_0$, heat conductivity $k_0$, the rate of heat production per unit mass $Q_0$, gravitational acceleration $g_0$, coefficient of thermal expansion $\alpha_0$, activation energy $E_0$, activation volume $V_0$, thermal diffusivity $\kappa_0 = k_0/(\rho_0 c_0)$, time $t_0 = l_0^2/\kappa_0$, velocity $u_0 = l_0/t_0$, and pressure $p_0 = g_0 l_0^2 c_0$.

We define new dimensionless variables and parameters (denoted by prime) as follows: $t = t' \cdot t_0$, $x = x' \cdot l_0$, $u = (u') \cdot u_0$, $T = T' \cdot T_0$, $p = p' \cdot p_0$, $\rho = \rho' \cdot \rho_0$, $\rho_0 = \rho_0' \cdot \rho_0$, $\mu = \mu' \cdot \mu_0$, $\mu_0 = \mu_0' \cdot \mu_0$, $g = g' \cdot g_0$, $\alpha = \alpha' \cdot \alpha_0$, $k = k' \cdot k_0$, $E = E' \cdot E_0$, $V = V' \cdot V_0$, $c = c' \cdot c_0$, and $Q = Q' \cdot Q_0$.

After the change of variables, the governing equations have the form

$$\text{Fr} \frac{\partial u}{\partial t} + \langle u, \nabla \rangle u = -\nabla p + \frac{1}{L_a} \text{div}(\mu e_{ij}) + F,$$

$$\frac{\partial}{\partial t}(\rho c T) + \langle u, \nabla (\rho c T) \rangle = \text{div}(k \nabla T) + \text{Di} \mu \Phi + \text{He} \rho Q,$$

$$\rho(t, x) = \rho_0(t, x)[1 - \alpha_0 T_0(T(t, x) - 1)],$$

$$\mu(t, x) = \mu_0(t, x) \text{exp}\left(\frac{E_0 E + \rho_0 g_0 l_0^3 \rho_0^2 V_0 V}{RT_0} - \frac{E_0 + \rho_0 g_0 l_0^3 V_0}{RT_0}\right),$$

$$\frac{\partial \rho_0}{\partial t} + \langle \nabla \rho_0, u \rangle = 0, \quad \frac{\partial u}{\partial t} + \langle \nabla \mu_0, u \rangle = 0.$$

These equations are written in terms of dimensionless variables and parameters. Hereafter, we omit the primes to simplify notation, which is thus made similar to the original dimensional notation. The equations contain the following dimensionless parameters:

$$\text{Fr} = \frac{\kappa_0^2}{g_0 l_0^2}, \quad L_a = \frac{\rho_0 g_0 l_0^3 \mu_0}{\kappa_0^2}, \quad \text{Di} = \frac{\mu_0 \kappa_0}{c_0 \rho_0 l_0^2}, \quad \text{He} = \frac{\rho_0 Q_0}{\kappa_0 T_0 c_0}.$$

Here, Fr is the Froude number, $Ra = \alpha_0 T_0 L_a$ is the Rayleigh number, Di is a parameter characterizing the rate of heat production due to the conversion of mechanical energy into internal energy through viscous friction, and He is a parameter characterizing the heat production due to other internal sources. Let us estimate these parameters by using the following characteristics of upper earth layers: $g_0 = 9.8 \text{ m s}^{-2}$, $\alpha_0 = 10^{-5} \text{ K}^{-1}$, $\rho_0 = 2.2 \times 10^3 \text{ kg m}^{-3}$, $\mu_0 = 10^{18} \text{ Pa s}$, $l_0 = 5 \times 10^{3} \text{ m}$, $k_0 = 3 \text{ J K}^{-1} \text{ m}^{-1} \text{ s}^{-1}$, $c_0 = 1250 \text{ J kg}^{-1} \text{ K}^{-1}$, $T_0 = 673 \text{ K}$,
The pressure \( p \) can be determined from (7) up to a constant. The components of \( \mathbf{u} = (u_1, u_2, u_3) \) can be calculated by using the equation \( \mathbf{u} = \text{curl} \mathbf{\psi} \) as

\[
\begin{align*}
u_1 &= \frac{\partial \psi_3}{\partial x_2} - \frac{\partial \psi_2}{\partial x_3}, \\
u_2 &= \frac{\partial \psi_1}{\partial x_3} - \frac{\partial \psi_3}{\partial x_1}, \\
u_3 &= \frac{\partial \psi_2}{\partial x_1} - \frac{\partial \psi_1}{\partial x_2}.
\end{align*}
\]
Equations (9)–(15) must be satisfied within the domain $\Omega$ at $t \geq t_0$. The functions $\psi_1$, $\psi_2$, $\psi_3$, and $T$ must satisfy the boundary conditions set on the boundary $\Gamma$ of $\Omega$. The functions $T$, $\rho_\#$, and $\mu_\#$ must satisfy initial conditions. We now proceed to formulating these conditions.

### 3. BOUNDARY AND INITIAL CONDITIONS

We set the initial moment at zero: $t_0 = 0$. For simplicity, the domain $\Omega$ is supposed to be a parallelepiped: $\Omega = (0, l_1) \times (0, l_2) \times (0, l_3)$. On the boundary $\Gamma$ of $\Omega$, which consists of the faces $\Gamma(x_i = 0)$ and $\Gamma(x_i = l_i)$ ($i = 1, 2, 3$), we set either impermeability conditions with perfect slip or no-slip conditions.

In the case of impermeability conditions with perfect slip, the velocity vector satisfies the following conditions at any $t \geq 0$:

$$\frac{\partial \mathbf{u}}{\partial n} = 0, \quad \langle \mathbf{u}, \mathbf{n} \rangle = 0 \quad \text{on} \quad \Gamma \text{ of } \Omega.$$

Here, $\mathbf{n}$ is the outward unit normal vector at a point on the boundary $\Gamma$, and $\mathbf{u}$ is the projection of the velocity vector onto the tangent plane at the same point on $\Gamma$.

In the case of no-slip conditions, the velocity vector satisfies the following condition at any $t \geq 0$:

$$\mathbf{u} = 0 \quad \text{on} \quad \Gamma \text{ of } \Omega.$$

Using the equation $\mathbf{u} = \nabla \times \mathbf{\psi}$, we write out the corresponding natural boundary conditions for $\mathbf{\psi}$. In the case of impermeability conditions with perfect slip, we have

$$\Gamma(x_1 = 0, x_1 = l_1) : \frac{\partial \psi_3}{\partial x_2} - \frac{\partial \psi_2}{\partial x_3} = 0, \quad \frac{\partial^2 \psi_1}{\partial x_1 \partial x_2} - \frac{\partial^2 \psi_3}{\partial x_1 \partial x_3} = 0 = \frac{\partial^2 \psi_2}{\partial x_1 \partial x_2} - \frac{\partial^2 \psi_1}{\partial x_1 \partial x_3},$$

$$\Gamma(x_2 = 0, x_2 = l_2) : \frac{\partial \psi_1}{\partial x_3} - \frac{\partial \psi_3}{\partial x_1} = 0, \quad \frac{\partial^2 \psi_2}{\partial x_1 \partial x_3} - \frac{\partial^2 \psi_3}{\partial x_1 \partial x_2} = 0 = \frac{\partial^2 \psi_1}{\partial x_1 \partial x_3} - \frac{\partial^2 \psi_2}{\partial x_1 \partial x_2},$$

$$\Gamma(x_3 = 0, x_3 = l_3) : \frac{\partial \psi_2}{\partial x_1} - \frac{\partial \psi_1}{\partial x_2} = 0, \quad \frac{\partial^2 \psi_3}{\partial x_1 \partial x_2} - \frac{\partial^2 \psi_1}{\partial x_1 \partial x_3} = 0 = \frac{\partial^2 \psi_2}{\partial x_1 \partial x_2} - \frac{\partial^2 \psi_3}{\partial x_1 \partial x_3}.$$

In the case of no-slip conditions, we have

$$\Gamma(x_1 = 0, x_1 = l_1) : \frac{\partial \psi_3}{\partial x_2} = \frac{\partial \psi_2}{\partial x_3} = 0, \quad \frac{\partial \psi_1}{\partial x_3} = \frac{\partial \psi_3}{\partial x_1} = 0, \quad \frac{\partial \psi_2}{\partial x_1} = \frac{\partial \psi_1}{\partial x_2} = 0,$$

$$\Gamma(x_2 = 0, x_2 = l_2) : \frac{\partial \psi_1}{\partial x_3} = \frac{\partial \psi_3}{\partial x_1} = 0, \quad \frac{\partial \psi_2}{\partial x_1} = \frac{\partial \psi_1}{\partial x_2} = 0, \quad \frac{\partial \psi_3}{\partial x_2} = \frac{\partial \psi_2}{\partial x_1} = 0,$$

$$\Gamma(x_3 = 0, x_3 = l_3) : \frac{\partial \psi_1}{\partial x_2} = \frac{\partial \psi_2}{\partial x_1} = 0, \quad \frac{\partial \psi_3}{\partial x_1} = \frac{\partial \psi_1}{\partial x_2} = 0, \quad \frac{\partial \psi_2}{\partial x_1} = \frac{\partial \psi_3}{\partial x_2} = 0.$$

However, we generally consider somewhat less specific and more restrictive boundary conditions for $\mathbf{\psi}$. This is done so that, when the variables in $\mathbf{\psi}$ are separated,

$$\psi_i = \psi_i(x_1, x_2, x_3) = \psi_i^{(1)}(x_1) \cdot \psi_i^{(2)}(x_2) \cdot \psi_i^{(3)}(x_3), \quad i = 1, 2, 3,$$

simple and natural boundary conditions are obtained for the multiplicands $\psi_i^{(1)}(x_1)$ in this tensor product.

In the case of impermeability conditions with perfect slip, the following more restrictive conditions are set:

$$\Gamma(x_1 = 0, x_1 = l_1) : \psi_2 = \psi_3 = 0, \quad \frac{\partial \psi_1}{\partial x_1} = 0, \quad \frac{\partial^2 \psi_2}{\partial x_1^2} = \frac{\partial^2 \psi_3}{\partial x_1^2} = 0,$$

$$\Gamma(x_2 = 0, x_2 = l_2) : \psi_1 = \psi_3 = 0, \quad \frac{\partial \psi_2}{\partial x_2} = 0, \quad \frac{\partial^2 \psi_1}{\partial x_2^2} = \frac{\partial^2 \psi_3}{\partial x_2^2} = 0,$$

$$\Gamma(x_3 = 0, x_3 = l_3) : \psi_1 = \psi_2 = 0, \quad \frac{\partial \psi_3}{\partial x_3} = 0, \quad \frac{\partial^2 \psi_1}{\partial x_3^2} = \frac{\partial^2 \psi_2}{\partial x_3^2} = 0.$$
\[ \Gamma(x_1 = 0, x_3 = l_3) : \psi_1 = \psi_2 = 0, \quad \frac{\partial \psi_1}{\partial x_3} = 0, \quad \frac{\partial^2 \psi_2}{\partial x_3^2} = \frac{\partial^2 \psi_2}{\partial x_3^2} = 0. \]

In the case of no-slip conditions, we set the following conditions:

\[ \Gamma(x_1 = 0, x_1 = l_1) : \psi_1 = \psi_2 = \psi_3 = 0, \quad \frac{\partial \psi_1}{\partial x_1} = \frac{\partial \psi_3}{\partial x_1} = 0, \]

\[ \Gamma(x_2 = 0, x_2 = l_2) : \psi_1 = \psi_2 = \psi_3 = 0, \quad \frac{\partial \psi_1}{\partial x_2} = \frac{\partial \psi_3}{\partial x_2} = 0, \]

\[ \Gamma(x_3 = 0, x_3 = l_3) : \psi_1 = \psi_2 = \psi_3 = 0, \quad \frac{\partial \psi_1}{\partial x_3} = \frac{\partial \psi_2}{\partial x_3} = 0. \]

For the temperature on the side faces on \( \Omega \), we set zero heat-flux conditions (as in a homogeneous Neumann problem). On the top and bottom faces of \( \Omega \), the following conditions for temperature are prescribed (as in a nonhomogeneous Dirichlet problem):

\[ \Gamma(x_1 = 0, x_1 = l_1) : \partial T/\partial x_1 = 0, \quad t \geq 0, \]

\[ \Gamma(x_2 = 0, x_2 = l_2) : \partial T/\partial x_2 = 0, \quad t \geq 0, \]

\[ \Gamma(x_3 = 0) : T(t, x_1, x_2, 0) = T_1(t, x_1, x_2), \quad t \geq 0, \]

\[ \Gamma(x_3 = l_3) : T(t, x_1, x_2, l_3) = T_2(t, x_1, x_2), \quad t \geq 0. \]

The initial conditions for temperature, density, and viscosity are set as follows:

\[ T(0, x) = T_0^0(x), \quad \rho_0^0(0, x) = \mu_0^0(x), \quad \mu_0^0(0, x) = \mu_0^0(x), \quad x \in \Omega. \]

Here, the prescribed functions \( T_0^0, \rho_0^0, \) and \( \mu_0^0 \) define the temperature and thermally unperturbed density and viscosity at the initial moment.

Equations (7)–(12), combined with the boundary and initial conditions, uniquely determine the unknown functions \( u_1, u_2, u_3, T, \rho, \) and \( \mu \) within \( \Omega \) at any \( t \geq 0 \). Equations (13)–(15) (with prescribed functions \( T, \rho_0, \) and \( \mu_0 \)) do not uniquely determine \( \psi_1, \psi_2, \) and \( \psi_3 \) under boundary conditions of any form. This is explained by the fact that \( \mathbf{u} \) can be expressed in terms of the corresponding vector potential \( \mathbf{\psi} \) only up to the gradient of an arbitrary differentiable scalar function \( \phi \), because \( \mathbf{u} = \nabla \times \mathbf{\psi} = \nabla (\mathbf{\psi} + \nabla \phi) \), which implies that \( \mathbf{u} = \nabla \psi_1 \) and \( \mathbf{u} = \nabla \psi_2 \), where \( \psi_1 = \psi_2 + \nabla \phi \). When a potential \( \mathbf{\psi} \) satisfies these relations, the potential \( \mathbf{\psi} + \nabla \phi \), where \( \phi \) is an arbitrary sufficiently smooth function of \( x \in \Omega \) with a compact support in \( \Omega \), satisfies these relations as well. Since \( \phi \) is a compactly supported function on \( \Omega \), the gradient \( \nabla \phi \) does not contribute to the boundary conditions for \( \mathbf{\psi} \). In particular, this implies that Eqs. (9)–(15), combined with the boundary and initial conditions, do not uniquely determine the unknown functions \( \psi_1, \psi_2, \) and \( \psi_3 \), whereas the unknown functions \( T, \rho_0, \) and \( \mu_0 \) (and, therefore, \( T, \rho, \) and \( \mu \)) are uniquely determined within \( \Omega \) at any \( t \geq 0 \).

For our purposes, any potential found by solving the equations above is suitable, because the same velocity field \( \mathbf{u} \) is obtained.

### 4. VARIATIONAL EQUATION OF THE PROBLEM

To apply a finite element method, we replace Eqs. (13)–(15) with an equivalent variational equation. We multiply Eqs. (13)–(15) by the components \( \omega \), of a test vector function \( \mathbf{\omega} \) satisfying the conditions set for the vector function \( \mathbf{\psi} \). Performing these operations and using the boundary conditions for the desired and test vector functions, we obtain the variational equation

\[ \int_{\Omega} \mu(2e_1\tilde{e}_{11} + 2e_{22}\tilde{e}_{22} + 2e_{33}\tilde{e}_{33} + e_{12}\tilde{e}_{12} + e_{13}\tilde{e}_{13} + e_{23}\tilde{e}_{23})dx = -La \int_{\Omega} \rho \omega_1 dx, \]

which can be compactly rewritten as

\[ E(\mathbf{\psi}, \mathbf{\omega}) = L(\mathbf{\omega}) \quad \text{for any admissible} \quad \mathbf{\omega} = (\omega_1, \omega_2, \omega_3). \]
Here, $E(\psi, \omega)$ and $L(\omega)$ denote the corresponding bilinear and linear forms. The expressions for $\ddot{e}_{ij}$ in terms of $\omega$ are identical to their expressions in terms of $\psi$.

The bilinear form $E(\psi, \omega)$ is symmetric:

$$E(\psi, \omega) = E(\omega, \psi)$$

for arbitrary admissible $\psi$ and $\omega$.

Moreover, it is nonnegative:

$$E(\omega, \omega) \geq 0$$

for any admissible $\omega$.

However, it is not positive definite; otherwise, the potential would be uniquely defined, which is not the case here, as shown above.

Thus, the problem is reduced to computing the functions $\psi_1 = \psi_1(t, x)$, $\psi_2 = \psi_2(t, x)$, $\psi_3 = \psi_3(t, x)$, $T = T(t, x)$, $\rho = \rho(t, x)$, and $\mu = \mu(t, x)$ that satisfy Eqs. (9)–(15) in the domain $\Omega$ at $t \geq 0$ (or the variational equation (17) combined with Eqs. (9)–(12)), supplemented with the boundary and initial conditions formulated above.

5. TWO-COMPONENT REPRESENTATION OF THE VECTOR POTENTIAL

Let us discuss the possibility of reducing the number of functions to be computed by reducing the number of required components of the vector potential $\psi$. Since numerical solution of the problem involves repeated computation of the flow velocity field (at different moments $t$) based on the corresponding current potential field, and the problem under analysis is three-dimensional, the reduction of the number of computed components of $\psi$ (say, from three to two) would result in a substantial economy of computing resources. This is a feasible task, because, as noted above, the vector potential is determined by the velocity field up to the gradient of a scalar function. Therefore, one can try to use the freedom in choosing a vector potential to accomplish this task.

We show here that, for a wide class of problems, it can be assumed a priori that $\psi_3 = 0$ in the required vector velocity potential $\psi$. To make this possible, we should find cases when the vector velocity field $\mathbf{u}$ admits the representation

$$\mathbf{u} = \text{curl} \psi, \quad \psi = (\psi_1, \psi_2, \psi_3), \quad \psi_3 = 0,$$

where the two-component potential $\psi = (\psi_1, \psi_2, 0)$ satisfies certain boundary conditions. The existence of such a representation would imply that the vector velocity potential could be sought in the two-component form and could be determined by solving either a simplified version of Eqs. (13)–(15) or a simplified variational equation derived from (17) under appropriately simplified boundary conditions with $\psi_3 = 0$. In what follows, we indicate some cases when this is possible.

Omitting a detailed analysis, we note the following fact verifiable by direct computation: for any sufficiently smooth vector field $\mathbf{u}$ satisfying only the incompressibility condition and an impermeability condition with either perfect slip or a no-slip condition, there exists a sufficiently smooth vector field $\psi$ that satisfies Eqs. (18) and the corresponding natural boundary conditions equivalent to impermeability with either perfect slip or no slip. As an example of such a $\psi$, consider the field defined by the following simple expressions:

$$\psi_1 = \psi_1(t, x_1, x_2, x_3) = \int_0^{x_1} u_3(t, x_1, x_2, \xi) d\xi + \frac{\partial \phi}{\partial x_1},$$

$$\psi_2 = \psi_2(t, x_1, x_2, x_3) = -\int_0^{x_2} u_1(t, x_1, x_2, \xi) d\xi + \frac{\partial \phi}{\partial x_2},$$

$$\psi_3 = \psi_3(t, x_1, x_2, x_3) = 0,$$

where $\phi = \phi(t, x_1, x_2)$ is an arbitrary, sufficiently smooth scalar function with a compact support in the rectangular domain $(0, l_1) \times (0, l_2)$ (the variable $t$ is treated here as a parameter). However, as mentioned above, it is more convenient from a computational perspective to deal with more restrictive boundary conditions for the velocity potential, because suitable basis functions are much easier to construct under such conditions in the finite element method to be used here in the approximate computation of the potential. In the analysis below, we use basis functions constructed from tricubic splines.
Now, let us explore the applicability of representation (18) under more restrictive boundary conditions for $\psi$. We begin with the case of more restrictive permeability conditions with perfect slip. We show here that the scalar function $\varphi$ in (19)–(21) can be adjusted so that the two-component potential defined by these expressions satisfy the more restrictive boundary conditions mentioned above. To do this, we need an additional condition: the velocity field must satisfy certain equations of state as well. In brief, this requirement can be substantiated as follows.

Consider a sufficiently smooth vector field $u$ satisfying the incompressibility condition (8), the permeability condition with perfect slip, and the equation of state (7) with admissible and sufficiently smooth $\rho = \rho(t, x)$, $\mu = \mu(t, x)$, and $p = p(t, x)$. Using the boundary conditions, we can represent the velocity field $u$ as Fourier series:

$$u_1(t, x_1, x_2, x_3) = \sum_{i = 0}^{\infty} \sum_{j = 0}^{\infty} \sum_{k = 0}^{\infty} u_{ijk}(t) \sin \frac{\pi i x_1}{l_1} \cos \frac{\pi j x_2}{l_2} \cos \frac{\pi k x_3}{l_3},$$

$$u_2(t, x_1, x_2, x_3) = \sum_{i = 0}^{\infty} \sum_{j = 0}^{\infty} \sum_{k = 0}^{\infty} u_{ijk}(t) \cos \frac{\pi i x_1}{l_1} \sin \frac{\pi j x_2}{l_2} \cos \frac{\pi k x_3}{l_3},$$

$$u_3(t, x_1, x_2, x_3) = \sum_{i = 0}^{\infty} \sum_{j = 0}^{\infty} \sum_{k = 0}^{\infty} u_{ijk}(t) \cos \frac{\pi i x_1}{l_1} \cos \frac{\pi j x_2}{l_2} \sin \frac{\pi k x_3}{l_3}.$$

Henceforth, the variable $t$ is treated as a parameter. The field $u$ can always be represented as $u = \text{curl} \psi$, where the three-component potential $\psi = (\psi_1, \psi_2, \psi_3)$ satisfies more restrictive boundary conditions. Using the boundary conditions, we represent the components of $\psi$ as Fourier series:

$$\psi_1(t, x_1, x_2, x_3) = \sum_{i = 0}^{\infty} \sum_{j = 0}^{\infty} \sum_{k = 0}^{\infty} \psi_{ijk}(t) \sin \frac{\pi i x_1}{l_1} \sin \frac{\pi j x_2}{l_2} \sin \frac{\pi k x_3}{l_3},$$

$$\psi_2(t, x_1, x_2, x_3) = \sum_{i = 0}^{\infty} \sum_{j = 0}^{\infty} \sum_{k = 0}^{\infty} \psi_{ijk}(t) \sin \frac{\pi i x_1}{l_1} \cos \frac{\pi j x_2}{l_2} \sin \frac{\pi k x_3}{l_3},$$

$$\psi_3(t, x_1, x_2, x_3) = \sum_{i = 0}^{\infty} \sum_{j = 0}^{\infty} \sum_{k = 0}^{\infty} \psi_{ijk}(t) \sin \frac{\pi i x_1}{l_1} \sin \frac{\pi j x_2}{l_2} \cos \frac{\pi k x_3}{l_3}.$$

Here, the Fourier coefficients obey the following constraints:

$$u_{ijk}(t) = \psi_{ijk}(t) \sin \frac{\pi i x_1}{l_1} \sin \frac{\pi j x_2}{l_2} \sin \frac{\pi k x_3}{l_3},$$

$$u_{ijk}(t) = \psi_{ijk}(t) \sin \frac{\pi i x_1}{l_1} \cos \frac{\pi j x_2}{l_2} \cos \frac{\pi k x_3}{l_3},$$

Substituting this representation of the vector potential into the variational equation (17) and consecutively using the test vector functions $\omega = (\omega_1, 0, 0)$, $\omega = (0, \omega_2, 0)$, and $\omega = (0, 0, \omega_3)$ with

$$\omega_1 = \cos \frac{\pi i x_1}{l_1} \sin \frac{\pi j x_2}{l_2} \sin \frac{\pi k x_3}{l_3}, \quad \omega_2 = \sin \frac{\pi i x_1}{l_1} \cos \frac{\pi j x_2}{l_2} \sin \frac{\pi k x_3}{l_3},$$

$$\omega_3 = \sin \frac{\pi i x_1}{l_1} \cos \frac{\pi j x_2}{l_2} \cos \frac{\pi k x_3}{l_3},$$

we obtain a system of linear equations that can be compactly written as

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \begin{pmatrix} \psi^{(1)} \\ \psi^{(2)} \\ \psi^{(3)} \end{pmatrix} = \begin{pmatrix} \rho^{(1)} \\ \rho^{(2)} \\ 0 \end{pmatrix}.$$
The entries of the infinite matrices $A_{pq}$ are constructed from the numbers
\[
a_{1ijk}^{1\text{lnn}} = (J^2 - K^2)(M^2 - N^2)\mu_{ijklmn}^{csc} + 4JMKN\mu_{ijklmn}^{ccc} + ILKN\mu_{ijklmn}^{ssc} + ILJM\mu_{ijklmn}^{ics},
\]
\[
a_{2ijk}^{1\text{lnn}} = LM(K^2 - L^2)\mu_{ijklmn}^{ics} - JJ(M^2 - N^2)\mu_{ijklmn}^{css} - 2JMKN\mu_{ijklmn}^{ccc} - JLMK\mu_{ijklmn}^{ics},
\]
\[
a_{1ijk}^{2\text{lnn}} = LN(J^2 - L^2)\mu_{ijklmn}^{csc} - JK(N^2 - L^2)\mu_{ijklmn}^{css} - 2JLMK\mu_{ijklmn}^{ccc} - ILMK\mu_{ijklmn}^{ics},
\]
\[
a_{2ijk}^{2\text{lnn}} = (J^2 - K^2)(L^2 - N^2)\mu_{ijklmn}^{csc} + 4ILKN\mu_{ijklmn}^{ccc} + JMK\mu_{ijklmn}^{ics} + ILJM\mu_{ijklmn}^{csc},
\]
\[
a_{3ijk}^{1\text{lnn}} = MN(I^2 - J^2)\mu_{ijklmn}^{css} - JK(N^2 - L^2)\mu_{ijklmn}^{csc} - 2JLMK\mu_{ijklmn}^{ccc} - ILMK\mu_{ijklmn}^{ics},
\]
\[
a_{3ijk}^{2\text{lnn}} = IK(M^2 - L^2)\mu_{ijklmn}^{csc} - LN(K^2 - J^2)\mu_{ijklmn}^{css} - 2IMKN\mu_{ijklmn}^{ccc} - ILMK\mu_{ijklmn}^{ics},
\]
\[
a_{3ijk}^{3\text{lnn}} = JK(L^2 - M^2)\mu_{ijklmn}^{csc} - MN(K^2 - I^2)\mu_{ijklmn}^{css} - 2ILJM\mu_{ijklmn}^{ccc} - ILJM\mu_{ijklmn}^{csc},
\]
\[
a_{3ijk}^{1\text{lnn}} = (I^2 - J^2)(L^2 - M^2)\mu_{ijklmn}^{csc} + 4ILJM\mu_{ijklmn}^{ccc} + JMK\mu_{ijklmn}^{ics} + ILJM\mu_{ijklmn}^{csc},
\]
where the following parameters are used:
\[
\mu_{ijklmn}^{csc} = \int \frac{\pi x_1}{l_1} \cos \frac{\pi x_1}{l_1} \cos \frac{\pi x_2}{l_2} \cos \frac{\pi x_3}{l_3} dx,
\]
\[
\mu_{ijklmn}^{css} = \int \frac{\pi x_1}{l_1} \cos \frac{\pi x_1}{l_1} \sin \frac{\pi x_2}{l_2} \sin \frac{\pi x_3}{l_3} dx,
\]
\[
\mu_{ijklmn}^{csc} = \int \frac{\pi x_1}{l_1} \sin \frac{\pi x_1}{l_1} \sin \frac{\pi x_2}{l_2} \cos \frac{\pi x_3}{l_3} dx,
\]
\[
\mu_{ijklmn}^{ics} = \int \frac{\pi x_1}{l_1} \sin \frac{\pi x_1}{l_1} \cos \frac{\pi x_2}{l_2} \cos \frac{\pi x_3}{l_3} dx,
\]
\[
I = \pi l_1, \quad J = \pi j/l_2, \quad K = \pi k/l_3, \quad L = \pi l_1, \quad M = \pi m/l_2, \quad N = \pi n/l_3.
\]

To formulate the rule for constructing $A_{pq}$ from $a_{pjk}^{q\text{lnn}}$, we introduce a one-dimensional indexing system for the equations and unknowns, using any one-to-one mapping $f: N_0 \times N_0 \times N_0 \mapsto N_0$, such that any triple index $(i, j, k) \in N_0 \times N_0 \times N_0$ is mapped to an index $f(i, j, k) \in N_0$, where $N_0 = \{0, 1, 2, \ldots\}$. The entries $(a_{p}^{q})_{ab}$ of a matrix $A_{pq}$ are now defined as $(a_{p}^{q})_{ab} = a_{bf(i, j, k)}^{q\text{lnn}}$, where $(l, m, n) = f^{-1}(a)$ and $(i, j, k) = f^{-1}(b)$.

The components of the vectors $\rho^{(1)}, \rho^{(2)}, \psi^{(1)}, \psi^{(2)}$, and $\psi^{(3)}$ are defined as
\[
\rho^{(1)}_{f(i, j, k)} = \frac{\pi m}{l_2} g \int \frac{\pi x_1}{l_1} \cos \frac{\pi x_1}{l_1} \cos \frac{\pi x_2}{l_2} \sin \frac{\pi x_3}{l_3} dx,
\]
\[
\rho^{(2)}_{f(i, j, k)} = \frac{\pi l}{l_1} g \int \frac{\pi x_1}{l_1} \cos \frac{\pi x_1}{l_1} \cos \frac{\pi x_2}{l_2} \sin \frac{\pi x_3}{l_3} dx,
\]
\[
\psi^{(1)}_{f(i, j, k)} = \psi^{(2)}_{f(i, j, k)}, \quad \psi^{(3)}_{f(i, j, k)} = \psi^{(3)}_{f(i, j, k)}, \quad \psi^{(3)}_{f(i, j, k)} = \psi^{(3)}_{f(i, j, k)}.
\]

If we multiply by $\pi l_1, \pi m/l_2$, and $\pi n/l_3$, respectively, each entry in the rows indexed by $f(l, m, n)$ in the sets of rows $(A_{11}, A_{12}, A_{13})$, $(A_{21}, A_{22}, A_{23})$, and $(A_{31}, A_{32}, A_{33})$ in (28) and add up the results, then we will
obtain a zero row, because
\[
\frac{\pi l}{l_1} a_{ijkl}^{(l,m,n)} + \frac{\pi m}{l_2} a_{ijkl}^{(j,k,l)} + \frac{\pi n}{l_3} a_{ijkl}^{(i,j,k)} = 0, \quad q = 1, 2, 3, \quad i, j, k, l, m, n \in N_0.
\]
As a result, we set to zero the last set of rows in the matrix of system (28). The last set of elements in the column of absolute terms will remain zero as well, because
\[
\frac{\pi l}{l_1} p^{(l,m,n)} + \frac{\pi m}{l_2} \rho^{(j,k,l)} + \frac{\pi n}{l_3} 0 = 0, \quad l, m, n \in N_0.
\]
This means that the vectors \(\psi^{(1)}, \psi^{(2)}, \) and \(\psi^{(3)}\) satisfy the system of linear equations
\[
\begin{pmatrix}
A_{11} & A_{12} & A_{13} \\
A_{21} & A_{22} & A_{23} \\
0 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
\psi^{(1)} \\
\psi^{(2)} \\
\psi^{(3)}
\end{pmatrix}
= \begin{pmatrix}
\rho^{(1)} \\
\rho^{(2)} \\
0
\end{pmatrix}.
\]
Moreover, the linear dependence of rows in the matrix of system (28) implies that systems (28) and (29) are equivalent. These systems are solvable since the vector field \(\psi\) satisfies the variational equation.

The columns of the matrices of systems (28) and (29) are also linearly dependent, because
\[
\frac{\pi l}{l_1} a_{ijkl}^{(l,m,n)} + \frac{\pi m}{l_2} a_{ijkl}^{(j,k,l)} + \frac{\pi n}{l_3} a_{ijkl}^{(i,j,k)} = 0, \quad p = 1, 2, 3, \quad i, j, k, l, m, n \in N_0.
\]
Therefore, the solvability of (29) entails the solvability of the system
\[
\begin{pmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{pmatrix}
\begin{pmatrix}
\psi^{(1)} \\
\psi^{(2)}
\end{pmatrix}
= \begin{pmatrix}
\rho^{(1)} \\
\rho^{(2)}
\end{pmatrix},
\]
and its solution is given by the vectors \(\psi^{(1)}\) and \(\psi^{(2)}\) whose components are
\[
\psi^{(1)}_{*f(i,k)} = \psi^{(1)}_{f(i,k)} - \frac{il_3}{k} \psi^{(3)}_{f(i,k)}, \quad \psi^{(2)}_{*f(i,k)} = \psi^{(2)}_{f(i,k)} - \frac{jl_2}{k} \psi^{(3)}_{f(i,k)},
\]
\[
i, j, k \in N_0, \quad k \neq 0,
\]
\[
\psi^{(1)}_{*f(i,0)} = 0, \quad \psi^{(2)}_{*f(i,0)} = 0, \quad i, j \in N_0.
\]
The reverse proposition is also valid: if vectors \(\psi^{(1)}\) and \(\psi^{(2)}\) constitute a solution to system (30), then the vectors \(\psi^{(1)} = \psi^{(1)}_{*}, \psi^{(2)} = \psi^{(2)}_{*}, \) and \(\psi^{(3)} = 0\) constitute a solution to both (28) and (29).

The analysis above implies that one may set \(\psi^{(3)} = 0\) when considering systems (28) and (29). Therefore, the velocity field \(u\) can be represented as in (18), where the potential \(\psi = (\psi_1, \psi_2, 0)\) satisfies the more restrictive boundary conditions corresponding to impermeability with perfect slip.

Now, we consider the case of no-slip conditions. The corresponding representation (18) subject to the more restrictive no-slip conditions is relatively simple to find when viscosity has the form \(\mu = \mu(t, x_3)\) or \(\mu = \mu(t, x_1, x_2)\). This assertion can be validated by an analysis that does not rely on the scheme developed above for the impermeability conditions with perfect slip. However, the desired representation (18) has been proved in the case when viscosity has the general form \(\mu = \mu(t, x)\) in [28] with the use of Chandrasekhar’s functions [16].

**Remark.** Note that the problem formulated for a horizontally uniform viscosity \(\mu = \mu(t, x_3)\) can be substantially simplified by replacing a three-component potential \(\psi = (\psi_1, \psi_2, \psi_3)\) or a two-component potential \(\psi = (\psi_1, \psi_2, 0)\) with the single-component potential
\[
\psi = \text{curl}(\phi e_3) = \left( \frac{\partial \phi}{\partial x_2}, -\frac{\partial \phi}{\partial x_1}, 0 \right),
\]
where \(\phi = \phi(t, x)\) is a scalar function satisfying appropriate boundary conditions. This can be done because the velocity field \(u\) can be represented as \(u = \text{curl} \, \text{curl}(\phi e_3)\) (note that this representation is not unique).
Omitting a detailed analysis, we note the scalar function $\varphi$ can be defined as a solution to the equation
\[ \frac{\partial^2 \varphi}{\partial x_1^2} + \frac{\partial^2 \varphi}{\partial x_2^2} = -u_3 \text{ in } \Omega. \]
In the case of impermeability conditions with perfect slip, this solution must satisfy the boundary conditions
\[
\Gamma(x_1 = 0, x_2 = l) : \varphi = 0, \quad \Gamma(x_1 = 0, x_2 = l) : \partial \varphi/\partial x_2 = 0, \\
\Gamma(x_1 = 0, x_2 = l) : \partial \varphi/\partial x_1 = 0.
\]
in the case of no-slip conditions, it must satisfy the boundary conditions
\[
\Gamma(x_1 = 0, x_2 = l) : \varphi = 0 = \partial \varphi/\partial x_1, \quad \Gamma(x_1 = 0, x_2 = l) : \varphi = 0 = \partial \varphi/\partial x_2, \\
\Gamma(x_1 = 0, x_2 = l) : \varphi = 0 = \partial \varphi/\partial x_3.
\]
Thus, the determination of $u$ for $u = \mu(t, x)$ can be reduced to computing a single scalar function $\varphi$ that satisfies both the corresponding simplified version of Eqs. (13)–(15) (or simplified variational equation (17)) and appropriate boundary conditions. In this case, it should be kept in mind that
\[
u_1 = -\partial^2 \varphi/\partial x_1 \partial x_3, \quad \nu_2 = \partial^2 \varphi/\partial x_2 \partial x_3, \quad \nu_3 = -\partial^2 \varphi/\partial x_1^2 - \partial^2 \varphi/\partial x_2^2.
\]

6. APPROXIMATION OF THE PROBLEM

Next, we consider some universal aspects of approximate solution of the basic equations for the desired functions. For example, the vector potential $\psi$ can be found, together with the thermally unperturbed density $\rho_\varphi$ and viscosity $\mu_\varphi$, by applying a finite element method with basis functions of a special form. The construction of the basis functions and the implementation of the finite element method were described in sufficient detail in [20–22]. Here, the vector potential is also approximated by a linear combination of tricubic basis functions expressed as tensor products of appropriate cubic splines:
\[
\psi_p(t, x_1, x_2, x_3) = \sum_{i=0}^{n_1} \sum_{j=0}^{n_2} \sum_{k=0}^{n_3} \psi_{ijk}^{(p)}(t) s_{ij}^{(p)}(x_1) s_{jk}^{(p)}(x_2) s_{ik}^{(p)}(x_3), \quad p = 1, 2. \tag{32}
\]
Density and viscosity are approximated by linear combinations of appropriate trilinear basis functions expressed as tensor products of linear functions:
\[
\rho_\varphi(t, x_1, x_2, x_3) = \sum_{i=0}^{n_1} \sum_{j=0}^{n_2} \sum_{k=0}^{n_3} \rho_{ijk}(t) s_{ij}^{(1)}(x_1) s_{jk}^{(2)}(x_2) s_{ik}^{(3)}(x_3), \tag{33}
\]
\[
\mu_\varphi(t, x_1, x_2, x_3) = \sum_{i=0}^{n_1} \sum_{j=0}^{n_2} \sum_{k=0}^{n_3} \mu_{ijk}(t) s_{ij}^{(1)}(x_1) s_{jk}^{(2)}(x_2) s_{ik}^{(3)}(x_3). \tag{34}
\]
Trilinear basis functions provide good approximations of discontinuous fluid properties.

By substituting approximations (32)–(34) into (17), the approximate vector potential is found for prescribed density and viscosity distributions by solving a system of linear algebraic equations with a positive definite band matrix for the unknown coefficients $\psi_{ijk}^{(p)}(t)$. However, the condition number of the system tends to infinity as the grid is condensed. This leads to difficulties in solving high-dimensional systems, since iterative methods tend to exhibit progressively slow convergence, and may even diverge in some cases because of roundoff errors. Here, a solution is obtained by directly applying the square-root method. Some versions of this method implemented on parallel computers were described and used in [20, 23–25].

Substituting approximations (33) and (34) into (12), we computed approximations of the thermally unperturbed density and viscosity for a prescribed velocity distribution by the method of characteristics, i.e., by transferring the initial conditions along the characteristics of Eqs. (12) (for details, see [20–22]). This method can be used in computations with relatively weak numerical diffusion of density and viscosity [20, 23, 26]. The characteristics of transport equations are defined by systems of ordinary differential equations of the form (see [18, 19, 26])
\[ dx(t)/dt = u(t, x(t)). \]
The thermally unperturbed density and viscosity have constant values on the characteristics:
\[ \rho_0(t, x(t)) = \rho_0(x(t_0)), \quad \mu_0(t, x(t)) = \mu_0(x(t_0)), \quad t \geq t_0. \]

These relations can be used to find density and viscosity in \( W \) at \( t > t_0 \) for the prescribed initial density and viscosity distributions, provided that the velocity fields at \( t \) have already been computed. When trilinear basis functions are used to approximate density and viscosity, a sufficiently large number of independent modules can be organized to compute the characteristics of transport equations and the corresponding densities and viscosities on them. Note that a finer grid can be used to approximate both density and viscosity, as compared to the grid used for computing the vector potential.

The temperature \( T = T(t, x) \) was approximated by finite-difference methods. The derivatives \( \partial u_i / \partial x_j \) were determined by differentiating the relation \( u = \text{curl} \psi \) with the use of (32). Temperature was computed by the implicit alternating-direction method [26]. At each iteration step in time, a large set of linear algebraic systems with tridiagonal matrices was solved, and a corresponding number of independent modules could be organized for parallel solution of these systems by means of tridiagonal algorithms.

In summary, the numerical solution of the problem consisted of the following basic stages: (1) a set of linear algebraic equations was solved for the coefficients of a decomposition of the vector velocity potential in terms of basis functions, (2) the heat equation was integrated, and (3) the transport equations for density and viscosity were integrated. All of these stages require substantial computing resources.

7. COMPUTATIONAL PROCEDURES

We briefly describe the procedures to be executed to solve the problem. A uniform discretization of the time axis, \( t_n = t_0 + \tau n \ (n \in \mathbb{Z}) \), is defined a priori, where \( \tau \) is the discretization parameter. Next, an iterative process is organized in which \( n \) is consecutively assigned integer values ranging from 0 to \( n \). (The integer
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Table

<table>
<thead>
<tr>
<th>Computer</th>
<th>Number of processors</th>
<th>CPU time</th>
<th>CPU type</th>
<th>Data transfer rate</th>
</tr>
</thead>
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<td>180''</td>
<td>I860/80 MHz</td>
<td>1 MB/s</td>
</tr>
<tr>
<td>MBC-1000</td>
<td>8</td>
<td>7''15''</td>
<td>Alpha/300 MHz</td>
<td>10 MB/s</td>
</tr>
<tr>
<td>Alpha</td>
<td>2</td>
<td>55''</td>
<td>Alpha/540 MHz</td>
<td>10 MB/s</td>
</tr>
<tr>
<td>IBM SP2</td>
<td>16</td>
<td>3''25''</td>
<td>RS6000/133 MHz</td>
<td>3 MB/s</td>
</tr>
</tbody>
</table>

$m$ is prescribed prior to computations to set the length of the interval $[t_0, t_m]$ of integration.) When necessary, the process can be continued further, starting from $t_m$ as an initial moment. At each iteration step in time, the following three steps are executed sequentially.

**Step 1.** The distributions of temperature, $T = T(t_n, \cdot)$, and thermally unperturbed density and viscosity, $\rho_0 = \rho_a(t_n, \cdot)$ and $\mu_0 = \mu_a(t_n, \cdot)$, at $t = t_n$ are used to determine from (10) and (11) the thermally perturbed $\rho = \rho(t_n, \cdot)$ and $\mu = \mu(t_n, \cdot)$ at the same $t = t_n$. Then, the distribution of $\psi = \psi(t_n, \cdot)$ is found by solving Eqs. (13)–(15) or variational equation (17), and (16) is used to calculate the velocity distribution $u = u(t_n, \cdot)$.

**Step 2.** The distributions of velocity, $u = u(t_n, \cdot)$, and thermally perturbed density and viscosity, $\rho = \rho(t_n, \cdot)$ and $\mu = \mu(t_n, \cdot)$, are used to compute a new temperature distribution $T = T(t_{n+1}, \cdot)$ at $t = t_{n+1}$ by solving Eq. (9) supplemented by boundary conditions.

**Step 3.** The distributions of velocity, $u = u(t_n, \cdot)$, and thermally unperturbed density and viscosity, $\rho_0 = \rho_a(t_n, \cdot)$ and $\mu_0 = \mu_a(t_n, \cdot)$, are used in (12) to compute new thermally unperturbed density and viscosity $\rho_0 = \rho_a(t_{n+1}, \cdot)$ and $\mu_0 = \mu_a(t_{n+1}, \cdot)$ at $t = t_{n+1}$.

The iterative process results in distributions of temperature $T = T(t_n, \cdot)$, potential $\psi = \psi(t_n, \cdot)$, velocity $u = u(t_n, \cdot)$, and thermally unperturbed density $\rho_0 = \rho_a(t_n, \cdot)$ and viscosity $\mu_0 = \mu_a(t_n, \cdot)$ at $t = t_n$ ($n = 0, 1, \ldots, m$). Once these distributions are available, the evolution of the system on the interval $[t_0, t_m]$ can be recovered in more detail by interpolation. The time step can be chosen automatically so that the largest displacement of fluid elements does not exceed a preset small amount.

8. NUMERICAL EXAMPLE

As a typical example, we computed a flow in the parallelepiped $\Omega = [0, 3] \times [0, 3] \times [0, 1]$. At $t_0 = 0$, we set $\rho_0^0(x) \equiv 1$, $\mu_0^0(x) \equiv 1$, and $T_0^0(x) = 1.05 - x_3/l_3$. On the faces $\Gamma(x_3 = l_3)$ and $\Gamma(x_3 = 0)$, we set $T_0(t, x) \equiv 0.05$ and $T_0(t, x) \equiv 1.05$, respectively. We set $Q = 0$ and restricted ourselves to the case of impermeability conditions with perfect slip. The values of physical parameters enumerated in Section 2 were adopted as characteristic of the upper earth layers. To kick the system out of an unstable equilibrium state, we introduced a small temperature disturbance at $x_0 = (3/2, 3/2, 1/3)$ at the initial moment, which led to the development of a diapir.

In computing the example, we used a $25 \times 25 \times 25$ grid for vector potential and viscosity, and a $73 \times 73 \times 73$ grid for density and temperature. The time step was set equal to 0.1. The table shows the processing characteristics of various parallel computers with distributed memory used to compute our numerical example.

The figure illustrates the variation of an isotherm computed at consecutive moments. The numerical results are consistent with those obtained in analyzing the development of Rayleigh–Bénard convection [16] and two-dimensional thermally driven convection [27].

CONCLUSIONS

We proposed a numerical approach to the problem of slow, highly viscous, incompressible flows with temperature-dependent density and viscosity involving gravitational and thermal effects. The approach relies on a finite element method and a representation of a two-component vector velocity potential for an incompressible viscous fluid by a linear combination of tricubic splines with unknown coefficients. The use of tricubic splines leads to a highly accurate solution to the problem, as compared to other finite-different or finite-element methods, while the discrete approximations employed have relatively low dimensions. The
transport equations for density and viscosity are solved by the method of characteristics; the heat balance equation, by means of a tridiagonal algorithm.

The two-component representation (18) of the vector velocity potential proposed in this study is computationally advantageous as compared to the two-component representation

\[ \mathbf{u} = \nabla \psi, \quad \psi = \nabla (\phi_1 \mathbf{e}_3) + \phi_2 \mathbf{e}_3, \]

with scalar poloidal and toroidal potentials \( \phi_1 \) and \( \phi_2 \) (e.g., see [9, 10, 16]). Representation (18) is simpler than (35). It entails simple relations (19)–(21) between the components of the velocity and potential vectors, which are equivalent to \( u_1 = -\partial \psi_2 / \partial x_3, \quad u_2 = \partial \psi_1 / \partial x_3, \quad u_3 = \partial \psi_2 / \partial x_1 - \partial \psi_1 / \partial x_2 \). When representation (35) is used, one has to deal with equations of higher order as compared to Eqs. (13)–(15), which require a more cumbersome and complicated numerical analysis. Moreover, representation (18) is valid not only in the domain \( \Omega \). It remains valid under the additional requirement that the boundary conditions considered here are consistently satisfied by the velocity vector and the corresponding vector potential. It is also important that the contributions previously made by various authors, including those published in [20–24], as well as available software, remain effective and may even turn out to be more efficient.

A greater part of computational resources is required to solve the system of linear algebraic equations obtained by discretizing the variational equation (17). The corresponding algorithm factorizes the matrix of the linear system and solves the resulting linear systems with upper and lower triangular matrices. The square root method is advantageous in that the solution is obtained up to the machine arithmetic accuracy. Its disadvantages include higher requirements for memory and CPU time resources. Iterative (e.g., Gauss–Seidel or Schwarz) methods require much less memory, but test computations have shown that the convergence rates of the iterative processes are too low. The multigrid iterative approach is also disadvantageous as applied to simulate thermally driven convection, since the corresponding convergence rate is too low when large variations of viscosity are to be computed [12, 13]. When the conjugate gradient method is applied, convergence cannot be improved to an acceptable degree, whereas the CPU time increases immensely [27]. It should be kept in mind that a high numerical accuracy is essential for computing the evolution of unstable flows, which are extremely sensitive to small disturbances (such as those resulting from numerical errors). This motivates the use of the highly accurate square root method for solving such problems. When the two-component velocity potential and, in some cases, the one-component potential proposed here are employed, the computing resources and CPU times required to solve the systems of equations are substantially reduced, and the basic disadvantage of the present approach is thereby eliminated.

The principal results of this study are summarized as follows:

1. A numerical method is developed for simultaneous solution of the Stokes flow equation, heat balance equation, and transport equations for physical parameters of the fluid.
2. It is demonstrated that computational costs can be reduced by reducing the dimensionality of the vector velocity potential.
3. Numerical results are obtained for some model problems in three-dimensional thermal convection.

ACKNOWLEDGMENTS

This work was supported by the International Science and Technology Center, project no. 1293-99 and by the Russian Foundation for Basic Research, project nos. 99-05-65050 and 99-07-90441.

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