

Appendix A

Algorithm for solving momentum equation

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Masanori Kameyama, Conditions for plate tectonics inferred from numerical experiments of mantle convection and shear zone formation, Ph.D thesis, University of Tokyo, 1998.

Since the Prandtl number, which is the ratio of kinematic viscosity to thermal diffusivity, of mantle material is significantly large, the inertia term disappears out of the equation of motion. This means that the equation of motion becomes an elliptic equation and that we must carry out a steady-state calculation for the equation of motion at every timestep. This is why a special treatment is necessary for calculations of mantle convection. In this section, we will show the algorithm employed in this study.

The mantle convection in a two-dimensional rectangular box is considered. We employed the staggered mesh system [Patankar, 1980]. The mesh system is shown in Figure A.1, where the thick solid lines indicate the boundaries of the region. We employ the control volume (CV) method [Patankar, 1980] in deriving discretized equations. In the followings, the numbers i and I denote indices in horizontal direction, while the numbers j and J denote indices in vertical direction; the indices i and j pass through the center of CV's and the I and J pass through the boundary of CV's. In this mesh system, the scalar field parameters, such as temperature, pressure, or, if any, chemical compositions, are defined at the center of meshes (i, j) , while the velocity components in x - and z -directions are defined at (I, j) and (i, J) , the center of mesh boundaries perpendicular to the axes, respectively.

A.1 Discretized equation for stream-function

In order to calculate the flow field, one should simultaneously solve the momentum and continuity equations. We solve the simultaneous equations by the use of stream-function ψ . In this section we obtain the discretized equation for ψ .

The partial differential equations describing the motion of fluid in x - and z -directions are

$$-\frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left(2\eta \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial z} \left[\eta \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \right] = 0, \quad (\text{A.1})$$

$$-\frac{\partial p}{\partial z} + \frac{\partial}{\partial x} \left[\eta \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \right] + \frac{\partial}{\partial z} \left(2\eta \frac{\partial w}{\partial z} \right) + \Delta\rho g = 0, \quad (\text{A.2})$$

respectively. Here, p is a pressure, η is viscosity of fluid, $\Delta\rho$ is density difference from surroundings, g is gravitational acceleration, and u and w are velocities in x - and z -directions, respectively. The z -axis is the vertical axis and positive upward. The partial differential form of continuity equation is

$$\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} = 0. \quad (\text{A.3})$$

The stream-function ψ is defined as,

$$u = \frac{\partial \psi}{\partial z}, \quad w = -\frac{\partial \psi}{\partial x}. \quad (\text{A.4})$$

Note that (A.4) automatically satisfy (A.3). By taking the rotation of (A.1) and (A.2) and substituting (A.4), we obtain a generalized biharmonic equation containing solely ψ as,

$$\left(\frac{\partial^2}{\partial z^2} - \frac{\partial^2}{\partial x^2} \right) \left[\eta \left(\frac{\partial^2 \psi}{\partial z^2} - \frac{\partial^2 \psi}{\partial x^2} \right) \right] + 4 \frac{\partial^2}{\partial x \partial z} \left(\frac{\partial^2 \psi}{\partial x \partial z} \right) = \frac{\partial}{\partial x} (\Delta\rho g). \quad (\text{A.5})$$

We discretize the partial differential equations (A.1) and (A.2) based on CV's shown in Figure A.2 and A.3, respectively. The mesh sizes and the grid intervals $dx_{(i)}$, $dz_{(j)}$, $\delta x_{(I)}$, and $\delta z_{(J)}$ are shown in the figures, and they are related to each other as,

$$\begin{aligned} \delta x_{(I)} &= \frac{1}{2} (dx_{(i-1)} + dx_{(i)}), \\ \delta z_{(J)} &= \frac{1}{2} (dz_{(j-1)} + dz_{(j)}). \end{aligned}$$

The discretized equations of (A.1), (A.2) and (A.3) are

$$\begin{aligned} \frac{p_{(i,j)} - p_{(i-1,j)}}{\delta x_{(I)}} &= \frac{1}{\delta x_{(I)}} \left[2\eta_{(i,j)} \frac{u_{(I+1,j)} - u_{(I,j)}}{dx_{(i)}} - 2\eta_{(i-1,j)} \frac{u_{(I,j)} - u_{(I-1,j)}}{dx_{(i-1)}} \right] \\ &+ \frac{1}{dz_{(j)}} \left[\eta_{g(I,J+1)} \frac{u_{(I,j+1)} - u_{(I,j)}}{\delta z_{(J+1)}} - \eta_{g(I,J)} \frac{u_{(I,j)} - u_{(I,j-1)}}{\delta z_{(J)}} \right] \\ &+ \frac{1}{dz_{(j)}} \left[\eta_{g(I,J+1)} \frac{w_{(i,J+1)} - w_{(i-1,J+1)}}{\delta x_{(I)}} - \eta_{g(I,J)} \frac{w_{(i,J)} - w_{(i-1,J)}}{\delta x_{(I)}} \right], \quad (\text{A.6}) \end{aligned}$$

$$\begin{aligned}
\frac{p(i,j) - p(i,j-1)}{\delta z(J)} &= \frac{1}{dx(i)} \left[\eta_{g(I+1,J)} \frac{w(i+1,J) - w(i,J)}{\delta x(I+1)} - \eta_{g(I,J)} \frac{w(i,J) - w(i-1,J)}{\delta x(I)} \right] \\
&+ \frac{1}{\delta z(J)} \left[2\eta_{(i,j)} \frac{w(i,J+1) - w(i,J)}{dz(j)} - 2\eta_{(i,j-1)} \frac{w(i,J) - w(i,J-1)}{dz(j-1)} \right] \\
&+ \frac{1}{dx(i)} \left[\eta_{g(I+1,J)} \frac{u(I+1,j) - u(I+1,j-1)}{\delta z(J)} - \eta_{g(I,J)} \frac{u(I,j) - u(I,j-1)}{\delta z(J)} \right] \\
&+ \Delta\rho g(i,J),
\end{aligned} \tag{A.7}$$

$$\frac{u(I+1,j) - u(I,j)}{dx(i)} + \frac{w(i,J+1) - w(i,J)}{dz(j)} = 0, \tag{A.8}$$

respectively. We eliminate p from (A.6) and (A.7) by taking the rotation as,

$$\begin{aligned}
0 &= (p(i,j) - p(i-1,j)) - (p(i,j-1) - p(i-1,j-1)) - (p(i,j) - p(i,j-1)) + (p(i-1,j) - p(i-1,j-1)) \\
&= 2\eta_{(i,j)} \frac{u(I+1,j) - u(I,j)}{dx(i)} - 2\eta_{(i-1,j)} \frac{u(I,j) - u(I-1,j)}{dx(i-1)} \\
&+ \eta_{g(I,J+1)} \frac{\delta x(I)}{dz(j)} \frac{u(I,j+1) - u(I,j)}{\delta z(J+1)} - \eta_{g(I,J)} \frac{\delta x(I)}{dz(j)} \frac{u(I,j) - u(I,j-1)}{\delta z(J)} \\
&+ \eta_{g(I,J+1)} \frac{1}{dz(j)} (w(i,J+1) - w(i-1,j+1)) - \eta_{g(I,J)} \frac{1}{dz(j)} (w(i,J) - w(i-1,J)) \\
&- 2\eta_{(i,j-1)} \frac{u(I+1,j-1) - u(I,j-1)}{dx(i)} + 2\eta_{(i-1,j-1)} \frac{u(I,j-1) - u(I-1,j-1)}{dx(i-1)} \\
&- \eta_{g(I,J)} \frac{\delta x(I)}{dz(j-1)} \frac{u(I,j) - u(I,j-1)}{\delta z(J)} + \eta_{g(I,J-1)} \frac{\delta x(I)}{dz(j-1)} \frac{u(I,j-1) - u(I,j-2)}{\delta z(J-1)} \\
&- \eta_{g(I,J)} \frac{1}{dz(j-1)} (w(i,J) - w(i-1,j)) + \eta_{g(I,J-1)} \frac{1}{dz(j-1)} (w(i,J-1) - w(i-1,J-1)) \\
&- \eta_{g(I+1,J)} \frac{\delta z(J)}{dx(i)} \frac{w(i+1,J) - w(i,J)}{\delta x(I+1)} + \eta_{g(I,J)} \frac{\delta z(J)}{dx(i)} \frac{w(i,J) - w(i-1,J)}{\delta x(I)} \\
&- 2\eta_{(i,j)} \frac{w(i,J+1) - w(i,J)}{dz(j)} + 2\eta_{(i,j-1)} \frac{w(i,J) - w(i,J-1)}{dz(j-1)} \\
&- \eta_{g(I+1,J)} \frac{1}{dx(i)} (u(I+1,j) - u(I+1,j-1)) + \eta_{g(I,J)} \frac{1}{dx(i)} (u(I,j) - u(I,j-1)) \\
&+ \eta_{g(I,J)} \frac{\delta z(J)}{dx(i-1)} \frac{w(i,J) - w(i-1,J)}{\delta x(I)} - \eta_{g(I-1,J)} \frac{\delta z(J)}{dx(i-1)} \frac{w(i-1,J) - w(i-2,J)}{\delta x(I-1)} \\
&+ 2\eta_{(i-1,j)} \frac{w(i-1,J+1) - w(i-1,J)}{dz(j)} - 2\eta_{(i-1,j-1)} \frac{w(i-1,J) - w(i-1,J-1)}{dz(j-1)} \\
&+ \eta_{g(I,J)} \frac{1}{dx(i-1)} (u(I,j) - u(I,j-1)) - \eta_{g(I-1,J)} \frac{1}{dx(i-1)} (u(I-1,j) - u(I-1,j-1)) \\
&- (\Delta\rho g(i,J) - \Delta\rho g(i-1,J)) \delta z(J).
\end{aligned} \tag{A.9}$$

We define the stream-function ψ in discretized form as,

$$u_{(I,j)} \equiv \frac{\psi_{(I,J+1)} - \psi_{(I,J)}}{dz(j)}, w_{(i,J)} \equiv -\frac{\psi_{(I+1,J)} - \psi_{(I,J)}}{dx(i)}, \tag{A.10}$$

Note that $\psi_{(I,J)}$ is chosen to automatically satisfy (A.8). Substituting (A.10) into (A.9), we obtain a discretized generalized biharmonic equation for ψ as,

$$(\Delta\rho g(i,J) - \Delta\rho g(i-1,J)) \delta z(J) =$$

$$\begin{aligned}
& \frac{\eta_{g(I,J-1)}}{dz_{(j-1)}} \times \left[\begin{aligned} & \frac{\delta x_{(I)}}{\delta z_{(j-1)}} \left(\frac{\psi_{(I,J)} - \psi_{(I,J-1)}}{dz_{(j-1)}} - \frac{\psi_{(I,J-1)} - \psi_{(I,J-2)}}{dz_{(j-2)}} \right) \\ & + \left(-\frac{\psi_{(I+1,J-1)} - \psi_{(I,J-1)}}{dx_{(i)}} + \frac{\psi_{(I,J-1)} - \psi_{(I-1,J-1)}}{dx_{(i-1)}} \right) \end{aligned} \right] \\
& + \frac{\eta_{g(I-1,J)}}{dx_{(i-1)}} \times \left[\begin{aligned} & \frac{\delta z_{(J)}}{\delta x_{(I-1)}} \left(\frac{\psi_{(I,J)} - \psi_{(I-1,J)}}{dx_{(i-1)}} - \frac{\psi_{(I-1,J)} - \psi_{(I-2,J)}}{dx_{(i-2)}} \right) \\ & + \left(-\frac{\psi_{(I-1,J+1)} - \psi_{(I-1,J)}}{dz_{(j)}} + \frac{\psi_{(I-1,J)} - \psi_{(I-1,J-1)}}{dz_{(j-1)}} \right) \end{aligned} \right] \\
& + \eta_{g(I,J)} \times 2 \left(\frac{1}{dx_{(i)} dx_{(i-1)}} - \frac{1}{dz_{(j)} dz_{(j-1)}} \right) \\
& \times \left[\begin{aligned} & \delta x_{(I)} \left(\frac{\psi_{(I,J+1)} - \psi_{(I,J)}}{dz_{(j)}} - \frac{\psi_{(I,J)} - \psi_{(I,J-1)}}{dz_{(j-1)}} \right) \\ & + \delta z_{(J)} \left(-\frac{\psi_{(I+1,J)} - \psi_{(I,J)}}{dx_{(i)}} + \frac{\psi_{(I,J)} - \psi_{(I-1,J)}}{dx_{(i-1)}} \right) \end{aligned} \right] \\
& + \frac{\eta_{g(I+1,J)}}{dx_{(i)}} \times \left[\begin{aligned} & \frac{\delta z_{(J)}}{\delta x_{(I+1)}} \left(\frac{\psi_{(I+2,J)} - \psi_{(I+1,J)}}{dx_{(i+1)}} - \frac{\psi_{(I+1,J)} - \psi_{(I,J)}}{dx_{(i)}} \right) \\ & + \left(-\frac{\psi_{(I+1,J+1)} - \psi_{(I+1,J)}}{dz_{(j)}} + \frac{\psi_{(I+1,J)} - \psi_{(I+1,J-1)}}{dz_{(j-1)}} \right) \end{aligned} \right] \\
& + \frac{\eta_{g(I,J+1)}}{dz_{(j)}} \times \left[\begin{aligned} & \frac{\delta x_{(I)}}{\delta z_{(j+1)}} \left(\frac{\psi_{(I,J+2)} - \psi_{(I,J+1)}}{dz_{(j+1)}} - \frac{\psi_{(I,J+1)} - \psi_{(I,J)}}{dz_{(j)}} \right) \\ & + \left(-\frac{\psi_{(I+1,J+1)} - \psi_{(I,J+1)}}{dx_{(i)}} + \frac{\psi_{(I,J+1)} - \psi_{(I-1,J+1)}}{dx_{(i-1)}} \right) \end{aligned} \right] \\
& + \frac{\eta_{(i-1,j-1)}}{dx_{(i-1)}} \times 4 \left[\frac{\psi_{(I,J)} - \psi_{(I,J-1)}}{dz_{(j-1)}} - \frac{\psi_{(I-1,J)} - \psi_{(I-1,J-1)}}{dz_{(j-1)}} \right] \\
& + \frac{\eta_{(i,j-1)}}{dx_{(i)}} \times 4 \left[-\frac{\psi_{(I+1,J)} - \psi_{(I+1,J-1)}}{dz_{(j-1)}} + \frac{\psi_{(I,J)} - \psi_{(I,J-1)}}{dz_{(j-1)}} \right] \\
& + \frac{\eta_{(i-1,j)}}{dx_{(i-1)}} \times 4 \left[-\frac{\psi_{(I,J+1)} - \psi_{(I,J)}}{dz_{(j)}} + \frac{\psi_{(I-1,J+1)} - \psi_{(I-1,J)}}{dz_{(j)}} \right] \\
& + \frac{\eta_{(i,j)}}{dx_{(i)}} \times 4 \left[\frac{\psi_{(I+1,J+1)} - \psi_{(I+1,J)}}{dz_{(j)}} - \frac{\psi_{(I,J+1)} - \psi_{(I,J)}}{dz_{(j)}} \right]. \tag{A.11}
\end{aligned}$$

Since we need to solve the above equation in terms of ψ , we rewrite (A.11) as an equation of ψ . We get the equation for ψ containing 13 values of ψ as,

$$\begin{aligned}
& a_{1(I,J)} \psi_{(I-2,J)} + a_{2(I,J)} \psi_{(I-1,J-1)} + a_{3(I,J)} \psi_{(I-1,J)} + a_{4(I,J)} \psi_{(I-1,J+1)} \\
& + a_{5(I,J)} \psi_{(I,J-2)} + a_{6(I,J)} \psi_{(I,J-1)} + a_{7(I,J)} \psi_{(I,J)} + a_{8(I,J)} \psi_{(I,J+1)} \\
& + a_{9(I,J)} \psi_{(I,J+2)} + a_{10(I,J)} \psi_{(I+1,J-1)} + a_{11(I,J)} \psi_{(I+1,J)} + a_{12(I,J)} \psi_{(I+1,J+1)} \\
& + a_{13(I,J)} \psi_{(I+2,J)} = b_{(I,J)}, \tag{A.12}
\end{aligned}$$

where

$$\begin{aligned}
a_{1(I,J)} &= \eta_{g(I-1,J)} \frac{\delta z_{(J)}}{dx_{(i-1)} dx_{(i-2)} \delta x_{(I-1)}}, \\
a_{2(I,J)} &= \frac{4\eta_{(i-1,j-1)} - \eta_{g(I,J-1)} - \eta_{g(I-1,J)}}{dx_{(i-1)} dz_{(j-1)}}, \\
a_{3(I,J)} &= \eta_{g(I-1,J)} \frac{2\delta z_{(J)}}{dx_{(i-1)}} \left(\frac{1}{dz_{(j)} dz_{(j-1)}} - \frac{1}{dx_{(i-1)} dx_{(i-2)}} \right) \\
&+ \eta_{g(I,J)} \frac{2\delta z_{(J)}}{dx_{(i-1)}} \left(\frac{1}{dz_{(j)} dz_{(j-1)}} - \frac{1}{dx_{(i)} dx_{(i-1)}} \right) \\
&- \frac{4\eta_{(i-1,j-1)}}{dx_{(i-1)} dz_{(j-1)}} - \frac{4\eta_{(i-1,j)}}{dx_{(i-1)} dz_{(j)}},
\end{aligned}$$

$$\begin{aligned}
a_{4(I,J)} &= \frac{4\eta_{(i-1,j)} - \eta_{g(I-1,J)} - \eta_{g(I,J+1)}}{dx_{(i-1)}dz_{(j)}}, \\
a_{5(I,J)} &= \eta_{g(I,J-1)} \frac{\delta x_{(I)}}{dz_{(j-1)}dz_{(j-2)}\delta z_{(J-1)}}, \\
a_{6(I,J)} &= \eta_{g(I,J-1)} \frac{2\delta x_{(I)}}{dz_{(j-1)}} \left(\frac{1}{dx_{(i)}dx_{(i-1)}} - \frac{1}{dz_{(j-1)}dz_{(j-2)}} \right) \\
&+ \eta_{g(I,J)} \frac{2\delta x_{(I)}}{dz_{(i-1)}} \left(\frac{1}{dx_{(i)}dx_{(i-1)}} - \frac{1}{dz_{(j)}dz_{(j-1)}} \right) \\
&- \frac{4\eta_{(i-1,j-1)}}{dx_{(i-1)}dz_{(j-1)}} - \frac{4\eta_{(i,j-1)}}{dx_{(i)}dz_{(j-1)}}, \\
a_{7(I,J)} &= \begin{matrix} a_{1(I,J)} & +a_{2(I,J)} & +a_{3(I,J)} & +a_{4(I,J)} & +a_{5(I,J)} & +a_{6(I,J)} \\ +a_{8(I,J)} & +a_{9(I,J)} & +a_{10(I,J)} & +a_{11(I,J)} & +a_{12(I,J)} & +a_{13(I,J)} \end{matrix} \\
&= \eta_{g(I,J-1)} \frac{\delta x_{(I)}}{dz_{(j-1)}^2\delta z_{(J-1)}} + \eta_{g(I-1,J)} \frac{\delta z_{(J)}}{dx_{(i-1)}^2\delta x_{(I-1)}} \\
&+ \eta_{g(I,J)} 4\delta x_{(I)}\delta z_{(J)} \left(\frac{1}{dx_{(i)}dx_{(i-1)}} - \frac{1}{dz_{(j)}dz_{(j-1)}} \right)^2 \\
&+ \eta_{g(I+1,J)} \frac{\delta z_{(J)}}{dx_{(i)}^2\delta x_{(I+1)}} + \eta_{g(I,J+1)} \frac{\delta x_{(I)}}{dz_{(j)}^2\delta z_{(J+1)}} \\
&+ \frac{4\eta_{(i-1,j-1)}}{dx_{(i-1)}dz_{(j-1)}} + \frac{4\eta_{(i,j-1)}}{dx_{(i)}dz_{(j-1)}} + \frac{4\eta_{(i-1,j)}}{dx_{(i-1)}dz_{(j)}} + \frac{4\eta_{(i,j)}}{dx_{(i)}dz_{(j)}}, \\
a_{8(I,J)} &= \eta_{g(I,J)} \frac{2\delta x_{(I)}}{dz_{(j)}} \left(\frac{1}{dx_{(i)}dx_{(i-1)}} - \frac{1}{dz_{(j)}dz_{(j-1)}} \right) \\
&+ \eta_{g(I,J+1)} \frac{2\delta x_{(I)}}{dz_{(j)}} \left(\frac{1}{dx_{(i)}dx_{(i-1)}} - \frac{1}{dz_{(j+1)}dz_{(j)}} \right) \\
&- \frac{4\eta_{(i-1,j)}}{dx_{(i-1)}dz_{(j)}} - \frac{4\eta_{(i,j)}}{dx_{(i)}dz_{(j)}}, \\
a_{9(I,J)} &= \eta_{g(I,J+1)} \frac{\delta x_{(I)}}{dz_{(j)}dz_{(j+1)}\delta z_{(J+1)}}, \\
a_{10(I,J)} &= \frac{4\eta_{(i,j-1)} - \eta_{g(I,J-1)} - \eta_{g(I+1,J)}}{dx_{(i)}dz_{(j-1)}}, \\
a_{11(I,J)} &= \eta_{g(I,J)} \frac{2\delta z_{(J)}}{dx_{(i)}} \left(\frac{1}{dz_{(j)}dz_{(j-1)}} - \frac{1}{dx_{(i)}dx_{(i-1)}} \right) \\
&+ \eta_{g(I+1,J)} \frac{2\delta z_{(J)}}{dx_{(i)}} \left(\frac{1}{dz_{(j)}dz_{(j-1)}} - \frac{1}{dx_{(i+1)}dx_{(i)}} \right) \\
&- \frac{4\eta_{(i,j-1)}}{dx_{(i)}dz_{(j-1)}} - \frac{4\eta_{(i,j)}}{dx_{(i)}dz_{(j)}}, \\
a_{12(I,J)} &= \frac{4\eta_{(i,j)} - \eta_{g(I+1,J)} - \eta_{g(I,J+1)}}{dx_{(i)}dz_{(j)}}, \\
a_{13(I,J)} &= \eta_{g(I+1,J)} \frac{\delta z_{(J)}}{dx_{(i)}dx_{(i+1)}\delta x_{(I+1)}}, \\
b_{(I,J)} &= (\Delta\rho g_{(i,J)} - \Delta\rho g_{(i-1,J)})\delta z_{(J)},
\end{aligned}$$

We solve the simultaneous equations (A.13) of $\psi_{(I,J)}$. In actual calculations, we write the equation (A.13) as an equation of matrices $\mathbf{Ax} = \mathbf{b}$. The coefficients $a_{1(I,J)}$ to $a_{13(I,J)}$ give all of the nonzero components of the matrix \mathbf{A} . Note that the coefficient matrix \mathbf{A} is a sparse and symmetric band matrix.

In this study, we solved the equation by the use of Gaussian elimination method modified for symmetric band matrices.¹

A.2 Incorporation of the boundary conditions

For simplicity, we assume the impermeable and shear-stress-free condition at all the boundaries. The conditions are written in partial differential form as,

$$\begin{aligned} u_{(x=0,z)} &= u_{(x=wd,z)} = \left(\frac{\partial w}{\partial z} \right)_{(x=0,z)} = \left(\frac{\partial w}{\partial z} \right)_{(x=wd,z)} = 0, \\ w_{(x,z=0)} &= w_{(x,z=d)} = \left(\frac{\partial u}{\partial x} \right)_{(x,z=0)} = \left(\frac{\partial u}{\partial x} \right)_{(x,z=d)} = 0, \end{aligned} \quad (\text{A.13})$$

where d is the height of the box and wd is the width of the box. The boundary conditions in discretized form are written as,

$$u_{(I=2,j)} = \frac{w_{(i=2,J)} - w_{(i=1,J)}}{\delta x_{(I=2)}} = 0 \quad \text{at left side wall} \quad (\text{A.14})$$

$$u_{(I=N_x+2,j)} = \frac{w_{(i=N_x+2,J)} - w_{(i=N_x+1,J)}}{\delta x_{(I=N_x+2)}} = 0 \quad \text{at right side wall} \quad (\text{A.15})$$

$$w_{(i,J=2)} = \frac{u_{(I,j=2)} - u_{(I,j=1)}}{\delta z_{(J=2)}} = 0 \quad \text{at bottom boundary} \quad (\text{A.16})$$

$$w_{(i,j=N_z+2)} = \frac{u_{(I,j=N_z+2)} - u_{(I,j=N_z+1)}}{\delta z_{(J=N_z+2)}} = 0 \quad \text{at top boundary} \quad (\text{A.17})$$

Substituting (A.10) we get boundary conditions for ψ as²,

$$\psi_{(I=1,J)} = -\psi_{(I=3,J)}, \quad \psi_{(I=2,J)} = 0 \quad \text{at left side wall } (x=0) \quad (\text{A.18})$$

$$\psi_{(I=N_x+3,J)} = -\psi_{(I=N_x+1,J)}, \quad \psi_{(I=N_x+2,J)} = 0 \quad \text{at right side wall } (x=wd) \quad (\text{A.19})$$

$$\psi_{(I,J=1)} = -\psi_{(I,J=3)}, \quad \psi_{(I,J=2)} = 0 \quad \text{at bottom boundary } (z=0) \quad (\text{A.20})$$

$$\psi_{(I,J=N_z+3)} = -\psi_{(I,J=N_z+1)}, \quad \psi_{(I,J=N_z+2)} = 0 \quad \text{at top boundary } (z=d) \quad (\text{A.21})$$

As can be seen from above, the independent components of $\psi_{(I,J)}$ are given by $3 \leq I \leq N_x + 1$ and $3 \leq J \leq N_z + 1$. When we build the discretized equation of $\psi_{(I,J)}$, we should incorporate the boundary condition for $I = 3, 4, N_x, N_x + 1$ and $J = 3, 4, N_z, N_z + 1$. For example, we consider the equation for $I = 3, 4$ (at left side wall). Letting $I = 3$ in (A.12) and substituting (A.18), we get

$$\begin{aligned} a_1 \times (-\psi_{(3,J)}) &+ a_2 \times 0 &+ a_3 \times 0 &+ a_4 \times 0 \\ + a_5 \psi_{(3,J-2)} &+ a_6 \psi_{(3,J-1)} &+ a_7 \psi_{(3,J)} &+ a_8 \psi_{(3,J+1)} \\ + a_9 \psi_{(3,J+2)} &+ a_{10} \psi_{(4,J-1)} &+ a_{11} \psi_{(4,J)} &+ a_{12} \psi_{(4,J+1)} \\ + a_{13} \psi_{(5,J)} &&&= b_{(3,J)}, \end{aligned} \quad (\text{A.22})$$

¹One can employ any other direct method in solving matrix equation of (A.13), such as LU decomposition and Cholesky decomposition. However, an iterative method like ICCG (Incomplete Cholesky decomposition plus Conjugate Gradient) is not suitable to solve a biharmonic equation of (A.13).

²Substitution of (A.10) into the boundary conditions for ψ only leads to,

$$\begin{aligned} \psi_{(I=2,J)} &= \psi_{(I=N_x+2,J)} = \text{const. for } \forall J, \\ \psi_{(I,J=2)} &= \psi_{(I,J=N_z+2)} = \text{const. for } \forall I. \end{aligned}$$

We chose the constants to be equal to zero in order to minimize the truncation error in solving ψ .

\Leftrightarrow

$$\begin{array}{cccc}
0 & +0 & +0 & +0 \\
+a_5\psi_{(3,J-2)} & +a_6\psi_{(3,J-1)} & +(a_7 - a_1)\psi_{(3,J)} & +a_8\psi_{(3,J+1)} \\
+a_9\psi_{(3,J+2)} & +a_{10}\psi_{(4,J-1)} & +a_{11}\psi_{(4,J)} & +a_{12}\psi_{(4,J+1)} \\
+a_{13}\psi_{(5,J)} & & & = b_{(3,J)},
\end{array} \tag{A.23}$$

The equation (A.23) is equivalent to (A.12) after the coefficients are modified as

$$a_{7(I=3,J)} \rightarrow a_{7(I=3,J)} - a_{1(I=3,J)}, \tag{A.24}$$

$$a_{1(I=3,J)} = a_{2(I=3,J)} = a_{3(I=3,J)} = a_{4(I=3,J)} = 0. \tag{A.25}$$

Letting $I = 4$ in (A.12) and substituting (A.18), we get

$$\begin{array}{cccc}
0 & +a_2\psi_{(3,J-1)} & +a_3\psi_{(3,J)} & +a_4\psi_{(3,J+1)} \\
+a_5\psi_{(4,J-2)} & +a_6\psi_{(4,J-1)} & +a_7\psi_{(4,J)} & +a_8\psi_{(4,J+1)} \\
+a_9\psi_{(4,J+2)} & +a_{10}\psi_{(5,J-1)} & +a_{11}\psi_{(5,J)} & +a_{12}\psi_{(5,J+1)} \\
+a_{13}\psi_{(6,J)} & & & = b_{(4,J)},
\end{array} \tag{A.26}$$

and this is equivalent to (A.12) with $a_{1(I=4,J)} = 0$.

After the similar consideration for $I = N_x, N_x + 1$ and $J = 3, 4, N_z, N_z + 1$, we obtain a complete set of boundary conditions as,

$$\begin{array}{l}
a_{7(I=3,J)} \rightarrow a_{7(I=3,J)} - a_{1(I=3,J)}, \\
a_{1(I=3,J)} = a_{2(I=3,J)} = a_{3(I=3,J)} = a_{4(I=3,J)} = 0, \quad \text{at left side wall} \\
a_{1(I=4,J)} = 0
\end{array} \tag{A.27}$$

$$\begin{array}{l}
a_{7(I=N_x+1,J)} \rightarrow a_{7(I=N_x+1,J)} - a_{1(I=N_x+1,J)}, \\
a_{1(I=N_x+1,J)} = a_{2(I=N_x+1,J)} = a_{N_x(I=N_x+1,J)} = a_{4(I=N_x+1,J)} = 0, \quad \text{at right side wall} \\
a_{13(I=N_x,J)} = 0
\end{array} \tag{A.28}$$

$$\begin{array}{l}
a_{7(I,J=3)} \rightarrow a_{7(I,J=3)} - a_{5(I,J=3)}, \\
a_{2(I,J=3)} = a_{5(I,J=3)} = a_{6(I,J=3)} = a_{10(I,J=3)} = 0, \quad \text{at bottom boundary} \\
a_{5(I,J=4)} = 0
\end{array} \tag{A.29}$$

$$\begin{array}{l}
a_{7(I,J=N_z+1)} \rightarrow a_{7(I,J=N_z+1)} - a_{9(I,J=N_z+1)}, \\
a_{4(I,J=N_z+1)} = a_{8(I,J=N_z+1)} = a_{9(I,J=N_z+1)} = a_{12(I,J=N_z+1)} = 0, \quad \text{at top boundary} \\
a_{9(I,J=N_z)} = 0
\end{array} \tag{A.30}$$

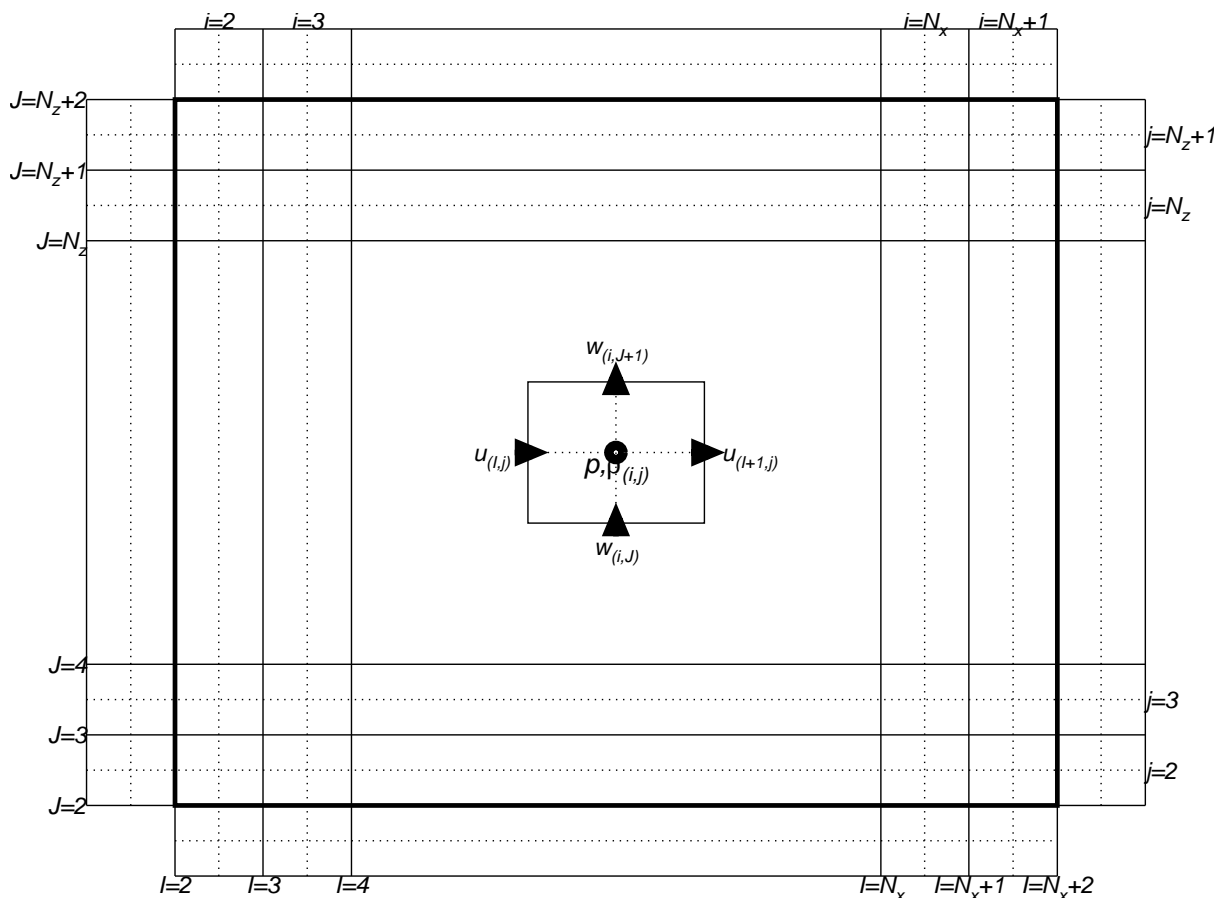
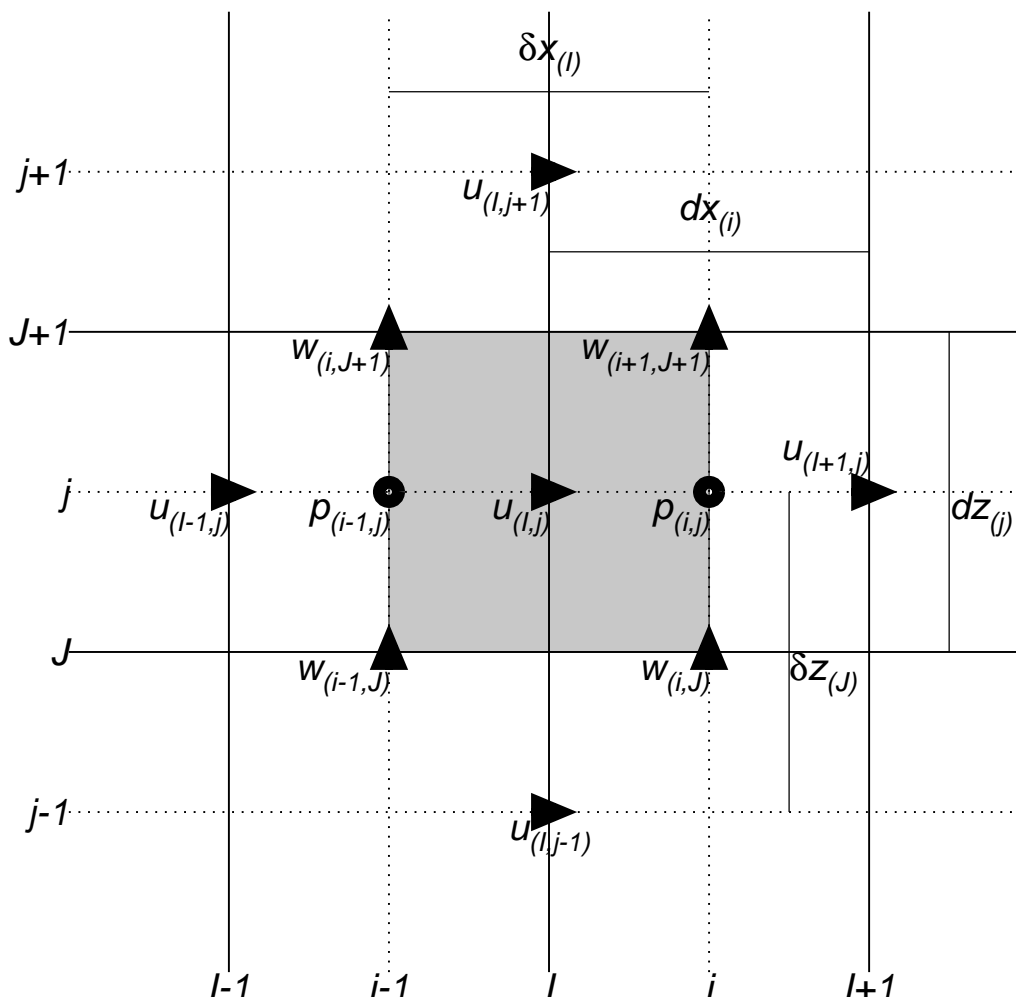
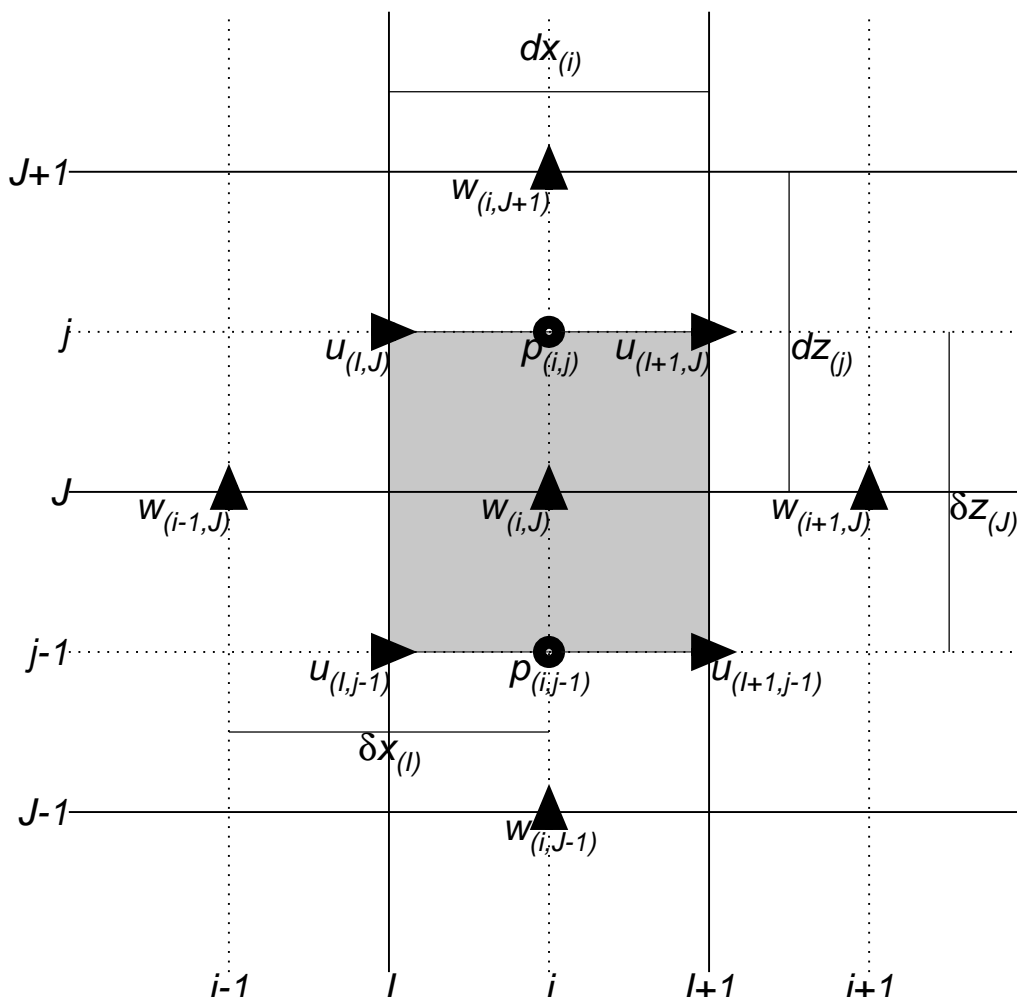


Figure A.1: The mesh system for mantle convection in two-dimensional rectangular box.

Figure A.2: Control volume for $u_{(I,j)}$.

Figure A.3: Control volume for $w_{(I,j)}$.