Mathematical Introduction to Geothermics and Geodynamics

(Lecture Notes)

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Chapter 1

Laws of conservation

In this chapter we shall formulate laws of conservation of mass, momentum and energy for a moving continuum. These basic laws will be employed throughout the whole textbook. Start with the two fundamental formulas:

The *Gauss theorem* is expressed in the formula

$$\int_{S(t)} \boldsymbol{h} \cdot \boldsymbol{n} \, dS = \int_{\Sigma(t)} [\boldsymbol{h}]_-^+ \cdot \boldsymbol{n} \, dS + \int_{V(t)\setminus\Sigma(t)} \nabla \cdot \boldsymbol{h}^T \, dV \, , \tag{1.1}$$

where $\boldsymbol{h}$ is a vector or tensor function continuously differentiable inside $V(t) \setminus \Sigma(t)$; $V(t)$ is a region in the continuum with a regular boundary $S(t)$ (see chapter ???) $\boldsymbol{n}$ is the outer normal to $S(t)$ or $\Sigma(t)$ and ^{T} means the transposition. $\Sigma(t)$ is an inner interface, where one of the two possible orientations of $\boldsymbol{n}$ is chosen as positive, and $[\boldsymbol{h}]_-^+ = \boldsymbol{h}^+ - \boldsymbol{h}^-$ denotes the jump of $\boldsymbol{h}$ across the interface obtained by subtracting its value on the negative side from that on the positive side. Finally, $\cdot$ represents the scalar product and t is time. We will consider below only the case, where the boundary $S(t)$ is formed by the same particles of continuum throughout the whole time interval taken into account. In other words $S(t)$ is "frozen" into the continuum.

Consequently, the *Reynolds transporting theorem* can be written as

$$\frac{D}{Dt} \int_{V(t)} f \, dV = \int_{V(t)\setminus\Sigma(t)} \left[\frac{\partial f}{\partial t} + \nabla \cdot (f \boldsymbol{v}) \right] \, dV + \int_{\Sigma(t)} [f(\boldsymbol{v} - \boldsymbol{\nu})]_-^+ \cdot \boldsymbol{n} \, dS \, , \tag{1.2}$$

where D/Dt is the material derivative, f represents a scalar, vector or tensor property of the continuum, $\boldsymbol{v}$ is the velocity of particles, whereas the velocity of the interface $\boldsymbol{\nu}$ may be, in general, different from the particle velocity. Both f and $\boldsymbol{v}$ are again required to be continuously differentiable inside $V(t) \setminus \Sigma(t)$.

1.1 Conservation of mass, momentum and moment of momentum

Since there is no mass flow through $S(t)$, the *law of mass conservation* can easily be expressed in the form

$$\frac{D}{Dt}\int_{V(t)} \rho \, dV = 0 \,, \tag{1.3}$$

where ρ represents the mass density. The Reynolds transporting theorem (1.2) yields

$$\int_{V(t)\setminus\Sigma(t)} \left[\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\boldsymbol{v})\right] dV + \int_{\Sigma(t)} [\rho(\boldsymbol{v}-\boldsymbol{\nu})]_-^+ \cdot \boldsymbol{n}\, dS = 0 \,. \tag{1.4}$$

The result must hold for arbitrary volume $V(t)$ (defined by its boundary $S(t)$) and thus both integrands must vanish. This is the reason why the integral (global) principle (1.4) can be replaced by a differential (local) principle

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\boldsymbol{v}) = 0 \quad \text{inside } V(t)\setminus\Sigma(t) \,, \tag{1.5}$$

which is usually called *the equation of continuity*, with the boundary condition

$$[\rho(\boldsymbol{v}-\boldsymbol{\nu})]_-^+ \cdot \boldsymbol{n} = 0 \quad \text{on } \Sigma(t) \,. \tag{1.6}$$

It should be noted that (1.6) does not represent a definition of a kind of an interface. For example, a chemical interface between two kinds of material is usually characterized by $\boldsymbol{v}=\boldsymbol{\nu}$ and the no-slip boundary is then defined by the simple relation $[\boldsymbol{v}]_-^+ = 0$. The integral principle (1.3) is more general than the equation of continuity (1.5) (complemented by the boundary condition (1.6)) since the integral principle does not require the existence of derivatives of density.

Combining (1.2) and (1.5) we get another useful formula

$$\frac{D}{Dt}\int_{V(t)} \rho f \, dV = \int_{V(t)\setminus\Sigma(t)} \left[\frac{\partial(\rho f)}{\partial t} + \nabla\cdot(\rho f\boldsymbol{v})\right] dV + \int_{\Sigma(t)} [\rho f(\boldsymbol{v}-\boldsymbol{\nu})]_-^+ \cdot \boldsymbol{n}\, dS =$$

$$\int_{V(t)\setminus\Sigma(t)} \left[\rho\frac{\partial f}{\partial t} + \rho\boldsymbol{v}\cdot\nabla f\right] dV + \int_{V(t)\setminus\Sigma(t)} \left[f\left(\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\boldsymbol{v})\right)\right] dV + \int_{\Sigma(t)} [\rho f(\boldsymbol{v}-\boldsymbol{\nu})]_-^+ \cdot \boldsymbol{n}\, dS =$$

$$= \int_{V(t)\setminus\Sigma(t)} \rho\frac{Df}{Dt}\, dV + \int_{\Sigma(t)} [\rho f(\boldsymbol{v}-\boldsymbol{\nu})]_-^+ \cdot \boldsymbol{n}\, dS \,. \tag{1.7}$$

The *law of momentum conservation* expresses a balance between changes of momentum and acting forces; its integral form is

$$\frac{D}{Dt}\int_{V(t)} \rho\boldsymbol{v}\, dV = \int_{V(t)} \rho\boldsymbol{g}\, dV - 2\int_{V(t)} \rho\boldsymbol{\Omega}\times\boldsymbol{v}\, dV - \int_{V(t)} \rho\boldsymbol{\Omega}\times(\boldsymbol{\Omega}\times\boldsymbol{r})\, dV + \int_{S(t)} \boldsymbol{\tau}\cdot\boldsymbol{n}\, dS \,, \tag{1.8}$$

where $\boldsymbol{g}$ is the gravity acceleration, $\boldsymbol{\Omega}$ is the angular frequency of the planet's rotation, $\boldsymbol{\tau}$ is the Cauchy stress tensor and $\times$ denotes the vector product. This means that we neglect all body forces except the gravitational, the Coriolis and the centrifugal forces. After applying (1.7) and (1.1) we will get

$$\int_{V(t)\setminus\Sigma(t)} \left[\rho\frac{D\boldsymbol{v}}{Dt} - \rho\boldsymbol{g} + 2\rho\boldsymbol{\Omega}\times\boldsymbol{v} + \rho\boldsymbol{\Omega}\times(\boldsymbol{\Omega}\times\boldsymbol{r}) - \nabla\cdot\boldsymbol{\tau}^T\right] dV$$

$$+ \int_{\Sigma(t)} [\rho\boldsymbol{v}(\boldsymbol{v}-\boldsymbol{\nu}) - \boldsymbol{\tau}]_-^+ \cdot \boldsymbol{n}\, dS = 0\,. \qquad (1.9)$$

Hence,

$$\nabla\cdot\boldsymbol{\tau}^T + \rho\boldsymbol{g} - 2\rho\boldsymbol{\Omega}\times\boldsymbol{v} - \rho\boldsymbol{\Omega}\times(\boldsymbol{\Omega}\times\boldsymbol{r}) = \rho\frac{D\boldsymbol{v}}{Dt} \equiv \rho(\frac{\partial\boldsymbol{v}}{\partial t} + \boldsymbol{v}\cdot\nabla\boldsymbol{v}) \quad \text{inside } V(t)\setminus\Sigma(t) \quad (1.10)$$

and

$$[\rho\boldsymbol{v}(\boldsymbol{v}-\boldsymbol{\nu}) - \boldsymbol{\tau}]_-^+ \cdot \boldsymbol{n} = 0 \quad \text{on } \Sigma(t)\,. \qquad (1.11)$$

Analogically, the law of conservation of moment of momentum can be written as

$$\frac{D}{Dt}\int_{V(t)} \boldsymbol{r}\times\rho\boldsymbol{v}\, dV = \int_{V(t)} \boldsymbol{r}\times\rho\boldsymbol{g}\, dV -$$

$$-2\int_{V(t)} \boldsymbol{r}\times(\rho\boldsymbol{\Omega}\times\boldsymbol{v})\, dV - \int_{V(t)} \boldsymbol{r}\times(\rho\boldsymbol{\Omega}\times(\boldsymbol{\Omega}\times\boldsymbol{r}))\, dV + \int_{S(t)} \boldsymbol{r}\times\boldsymbol{\tau}\cdot\boldsymbol{n}\, dS\,, \quad (1.12)$$

where $\boldsymbol{r}$ is the radius vector. Since $\int_{V(t)} \boldsymbol{r}\times\rho\boldsymbol{v}\, dV = \int_{V(t)} \rho[\boldsymbol{r}\times\boldsymbol{v}]\, dV$, $\frac{D}{Dt}(\boldsymbol{r}\times\boldsymbol{v}) = \boldsymbol{r}\times\frac{D\boldsymbol{v}}{Dt}$, $\nabla\boldsymbol{r} = \boldsymbol{I}$ ($\boldsymbol{I}$ is the identity tensor) and $[\boldsymbol{r}]_-^+ = 0$, the application of (1.7) and (1.1) to (1.12) now leads to

$$\int_{V(t)\setminus\Sigma(t)} \boldsymbol{r}\times\left(\rho\frac{D\boldsymbol{v}}{Dt} - \rho\boldsymbol{g} + 2\rho\boldsymbol{\Omega}\times\boldsymbol{v} + \rho\boldsymbol{\Omega}\times(\boldsymbol{\Omega}\times\boldsymbol{r}) - \nabla\cdot\boldsymbol{\tau}^T\right) dV -$$

$$-\int_{V(t)\setminus\Sigma(t)} \boldsymbol{I}\dot{\times}\boldsymbol{\tau}\, dV + \int_{\Sigma(t)} \boldsymbol{r}\times[\rho\boldsymbol{v}(\boldsymbol{v}-\boldsymbol{\nu}) - \boldsymbol{\tau}]_-^+ \cdot\boldsymbol{n}\, dS = 0\,, \qquad (1.13)$$

where $\dot{\times}$ is the double product consisting of vector and scalar products. [1] By virtue of (1.10) and (1.11) we have

$$\boldsymbol{I}\dot{\times}\boldsymbol{\tau} = 0 \iff \boldsymbol{\tau} = (\boldsymbol{\tau})^T\,, \qquad (1.14)$$

i.e. $\boldsymbol{\tau}$ is a symmetric tensor and thus the transposition in (1.10) may be omitted.

[1] In Cartesian coordinates $\boldsymbol{I}\dot{\times}\boldsymbol{\tau} = \sum_{jk} \epsilon_{ijk}\delta_{jl}\tau_{kl}$, δ_{jl} is the Kronecker δ-symbol and ϵ_{ijk} is the Levi-Civita permutation symbol.

1.2 Conservation of energy

The principle of conservation of energy can be expressed in the form,

$$\frac{D}{Dt}\int_V (\rho\epsilon + \frac{1}{2}\rho\boldsymbol{v}\cdot\boldsymbol{v})\,dV =$$

$$= \int_{S(t)} \boldsymbol{v}\cdot\boldsymbol{\tau}\cdot\boldsymbol{n}\,dS + \int_{V(t)} \rho\boldsymbol{g}\cdot\boldsymbol{v}\,dV - 2\int_{V(t)} \rho(\boldsymbol{\Omega}\times\boldsymbol{v})\cdot\boldsymbol{v}\,dV - \int_{V(t)} \rho(\boldsymbol{\Omega}\times(\boldsymbol{\Omega}\times\boldsymbol{r}))\cdot\boldsymbol{v}\,dV - \tag{1.15}$$

$$- \int_S \boldsymbol{q}\cdot\boldsymbol{n}\,dS + \int_V H\,dV\,,$$

where ϵ is an internal energy per unit mass, $\boldsymbol{q}$ represents the heat flow and H denotes the heat sources per unit volume. Note that the first term on the right-hand side of this energy balance equation is a work produced by surfaces forces per unit time, the three following terms describe the work produced by the considered body forces (gravity, Coriolis and centrifugal). However, $\boldsymbol{v}$ is perpendicular to $\boldsymbol{\Omega}\times\boldsymbol{v}$ and thus the Coriolis force does not produce any work. Let us denote these terms by

$$\mathcal{E} = \int_{S(t)} \boldsymbol{v}\cdot\boldsymbol{\tau}\cdot\boldsymbol{n}\,dS + \int_{V(t)} \rho\boldsymbol{g}\cdot\boldsymbol{v}\,dV - \int_{V(t)} \rho(\boldsymbol{\Omega}\times(\boldsymbol{\Omega}\times\boldsymbol{r}))\cdot\boldsymbol{v}\,dV - \frac{D}{Dt}\int_{V(t)} \frac{1}{2}\rho\boldsymbol{v}\cdot\boldsymbol{v}\,dV\,. \tag{1.16}$$

It holds

$$\int_{S(t)} \boldsymbol{v}\cdot\boldsymbol{\tau}\cdot\boldsymbol{n}\,dS = \int_{V(t)\setminus\Sigma(t)} [\boldsymbol{v}\cdot(\nabla\cdot\boldsymbol{\tau}) + \nabla\boldsymbol{v} : \boldsymbol{\tau}]\,dV + \int_{\Sigma(t)} [\boldsymbol{v}\cdot\boldsymbol{\tau}]_-^+\cdot\boldsymbol{n}\,dS\,, \tag{1.17}$$

where : denotes the double scalar product. [2] Since $\rho\frac{D\boldsymbol{v}}{Dt}\cdot\boldsymbol{v} = \frac{1}{2}\rho\frac{D}{Dt}(\boldsymbol{v}\cdot\boldsymbol{v})$, (1.10) yields

$$\int_{V(t)\setminus\Sigma(t)} \boldsymbol{v}\cdot(\nabla\cdot\boldsymbol{\tau})\,dV =$$

$$= \int_{V(t)\setminus\Sigma(t)} \frac{1}{2}\rho\frac{D}{Dt}(\boldsymbol{v}\cdot\boldsymbol{v})\,dV - \int_{V(t)} \rho\boldsymbol{g}\cdot\boldsymbol{v}\,dV + \int_{V(t)} \rho(\boldsymbol{\Omega}\times(\boldsymbol{\Omega}\times\boldsymbol{r}))\cdot\boldsymbol{v}\,dV\,. \tag{1.18}$$

Hence, after putting $-\frac{D}{Dt}\int_{V(t)}\frac{1}{2}\rho\boldsymbol{v}\cdot\boldsymbol{v}\,dV = -\int_{V(t)\setminus\Sigma(t)}\frac{1}{2}\rho\frac{D}{Dt}(\boldsymbol{v}\cdot\boldsymbol{v})\,dV -$
$-\int_{\Sigma(t)}\left[\frac{1}{2}\rho(\boldsymbol{v}\cdot\boldsymbol{v})(\boldsymbol{v}-\boldsymbol{\nu})\right]_-^+\cdot\boldsymbol{n}\,dS$ into (1.16), we get

$$\mathcal{E} = \int_{V(t)\setminus\Sigma(t)} \boldsymbol{\tau} : \nabla\boldsymbol{v}\,dV + \int_{\Sigma(t)} [\boldsymbol{v}\cdot\boldsymbol{\tau}]_-^+\cdot\boldsymbol{n}\,dS - \int_{\Sigma(t)} [\frac{1}{2}\rho(\boldsymbol{v}\cdot\boldsymbol{v})(\boldsymbol{v}-\boldsymbol{\nu})]_-^+\cdot\boldsymbol{n}\,dS\,. \tag{1.19}$$

After applying (1.1) to $-\int_S \boldsymbol{q}\cdot\boldsymbol{n}\,dS$ and (1.7) to $\frac{D}{Dt}\int_V \rho\epsilon\,dV$, we finally get

$$\rho\frac{D\epsilon}{Dt} = -\nabla\cdot\boldsymbol{q} + \boldsymbol{\tau} : \nabla\boldsymbol{v} + H \quad \text{inside } V(t)\setminus\Sigma(t)\,, \tag{1.20}$$

[2] In Cartesian coordinates $\nabla\boldsymbol{v} : \boldsymbol{\tau} = \sum_{ij}\frac{\partial v_i}{\partial x_j}\tau_{ij}$.

$$[\boldsymbol{q}]_-^+ \cdot \boldsymbol{n} = [\boldsymbol{v}\cdot\boldsymbol{\tau}]_-^+ \cdot \boldsymbol{n} - [(\rho\epsilon + \frac{1}{2}\rho\boldsymbol{v}\cdot\boldsymbol{v})(\boldsymbol{v}-\boldsymbol{\nu})]_-^+ \cdot \boldsymbol{n} \quad \text{on } \Sigma(t)\,. \tag{1.21}$$

In the Earth, a substantial part R of internal heating is caused by a decay of radioactive isotopes, i.e.

$$H = R + H'\,, \tag{1.22}$$

$$R = \rho\sum_i Z_i c_i e^{-\frac{t}{\lambda_i}}\,, \tag{1.23}$$

where Z_i is the heat production of 1 kg of pure i-th radioactive element per 1 sec, c_i is the mass concentration of the sum of "mother" and "daughter" isotopes and λ_i^{-1} is the rate constant of decay. [3] However, if we do not consider diffusion of atoms of radioactive isotopes and the mass changes during decays, the equation of continuity (1.5) as well as the boundary condition (1.6) hold also for ρc_i, i.e.

$$\frac{\partial R}{\partial t} + \nabla\cdot(R\boldsymbol{v}) = \sum_i\left[-\rho c_i\frac{Z_i}{\lambda_i}e^{-\frac{t}{\lambda_i}} + \frac{\partial(\rho c_i)}{\partial t}Z_i e^{-\frac{t}{\lambda_i}} + \nabla\cdot(\rho c_i\boldsymbol{v})Z_i e^{-\frac{t}{\lambda_i}}\right] = -\sum_i \rho c_i\frac{Z_i}{\lambda_i}e^{-\frac{t}{\lambda_i}}\,. \tag{1.24}$$

We will consider now that the continuum is *a classical viscous heat-conducting fluid.* Then it holds,

$$\boldsymbol{\tau} = -p\boldsymbol{I} + \boldsymbol{\sigma}(\boldsymbol{v})\,, \quad \lim_{\boldsymbol{v}\to 0}\boldsymbol{\sigma}(\boldsymbol{v}) = 0\,, \tag{1.25}$$

where p is the thermodynamic pressure [4], and

$$\boldsymbol{q} = -\boldsymbol{k}\cdot\nabla T\,, \tag{1.26}$$

where $\boldsymbol{k}$ is the thermal conductivity tensor and T is the absolute temperature. Now we will employ the Gibbs relation

$$\rho T\frac{Ds}{Dt} = \rho\frac{D\epsilon}{Dt} + p\nabla\cdot\boldsymbol{v}\,, \tag{1.27}$$

where s is the entropy per unit mass (for the details see section 6.2 and, especially, the relation (6.34) in the lecture notes on continuum mechanics by Z. Martinec). If we employ the energy balance (1.20), (1.21), we obtain the heat transfer equation expressed by means of entropy in the form:

$$\rho T\frac{Ds}{Dt} = \nabla\cdot(\boldsymbol{k}\cdot\nabla T) + \boldsymbol{\sigma} : \nabla\boldsymbol{v} + H \quad \text{inside } V(t)\setminus\Sigma(t)\,, \tag{1.28}$$

where $\boldsymbol{\sigma} : \nabla\boldsymbol{v}$ is the *dissipation* of heat,

$$[\boldsymbol{k}\cdot\nabla T]_-^+ \cdot \boldsymbol{n} = -[\boldsymbol{v}\cdot\boldsymbol{\tau}]_-^+ \cdot \boldsymbol{n} + [(\rho\epsilon + \frac{1}{2}\rho\boldsymbol{v}\cdot\boldsymbol{v})(\boldsymbol{v}-\boldsymbol{\nu})]_-^+ \cdot \boldsymbol{n} \quad \text{on } \Sigma(t)\,. \tag{1.29}$$

[3] We characterize each decay series by means of only one rate constant.

[4] In general, $\boldsymbol{\sigma}$ is not a deviatoric part of $\boldsymbol{\tau}$, i.e., $p \neq -\frac{1}{3}\sum_i \tau_{ii}$.

1.3 Heat equation expressed by means of the state variables

A state of classical viscous heat-conducting fluid is determined by means of the three state variables — the absolute temperature T, the pressure p and the volume V. In what follows, we will consider a fluid of unit mass, i.e., $V = 1/\rho$. These three variables are not independent because the thermodynamic properties of the medium are given by the *equation of state*, which may be formally written as

$$f(p, T, V) = 0\,. \tag{1.30}$$

Usually, we will consider it in the form

$$\rho = \rho(p, T)\,. \tag{1.31}$$

Therefore, only two variables may be independent.

1.3.1 Heat equation in T, V variables

If we choose temperature and volume as independent variables, we must express the dependence of entropy s on T and V. We may derive

$$\rho T \frac{Ds}{Dt} = \rho T \left(\frac{\partial s}{\partial T}\right)_V \frac{DT}{Dt} + \rho T \left(\frac{\partial s}{\partial V}\right)_T \frac{DV}{Dt} = \rho c_v \frac{DT}{Dt} - \frac{\mu}{\rho}\frac{D\rho}{Dt} = \rho c_v \frac{DT}{Dt} + \mu \nabla \cdot \boldsymbol{v}\,,^{5} \tag{1.32}$$

where c_v is the isochoric specific heat and $\mu \equiv T\left(\frac{\partial s}{\partial V}\right)_T$. In what follows, we will try to express μ by means of measurable quantities. The second and first thermodynamic laws are

$$T\,ds = T\left(\frac{\partial s}{\partial T}\right)_V dT + T\left(\frac{\partial s}{\partial V}\right)_T dV = c_v\,dT + \mu\,dV\,, \tag{1.33}$$

$$T\,ds = dU + p\,dV = \left(\frac{\partial U}{\partial T}\right)_V dT + \left[\left(\frac{\partial U}{\partial V}\right)_T + p\right] dV = c_v\,dT + \mu\,dV\,. \tag{1.34}$$

The second thermodynamic law (1.33) implies

$$\left(\frac{\partial c_v}{\partial V}\right)_T - \left(\frac{\partial \mu}{\partial T}\right)_V = -\left(\frac{\partial s}{\partial V}\right)_T = -\frac{\mu}{T} \tag{1.35}$$

but the first thermodynamic law (1.34) yields

$$\left(\frac{\partial c_v}{\partial V}\right)_T - \left(\frac{\partial \mu}{\partial T}\right)_V = -\left(\frac{\partial p}{\partial T}\right)_V \tag{1.36}$$

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[5] $\frac{D\rho}{Dt} = \frac{\partial \rho}{\partial t} + \boldsymbol{v}\cdot\nabla\rho = \frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\boldsymbol{v}) - \rho\nabla\cdot\boldsymbol{v} = -\rho\nabla\cdot\boldsymbol{v}$

and thus the combination of (1.35) and (1.36) gives

$$\mu = T \left(\frac{\partial p}{\partial T}\right)_V . \tag{1.37}$$

An isochoric basic equation is

$$dV \equiv \left(\frac{\partial V}{\partial p}\right)_T dp + \left(\frac{\partial V}{\partial T}\right)_p dT = 0 \tag{1.38}$$

and thus

$$\left(\frac{\partial p}{\partial T}\right)_V = -\left(\frac{\partial V}{\partial T}\right)_p \left(\frac{\partial p}{\partial V}\right)_T = \left[\frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p\right]\left[-V\left(\frac{\partial p}{\partial V}\right)_T\right] \equiv \alpha K_T \, , \tag{1.39}$$

where $\alpha \equiv \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_p$ is the thermal expansion coefficient and $K_T \equiv -V\left(\frac{\partial p}{\partial V}\right)_T = \rho\left(\frac{\partial p}{\partial \rho}\right)_T$ is the isothermal bulk modulus. Carrying (1.39) into (1.37), we get

$$\mu = T \alpha K_T \equiv \rho c_v T \gamma \, , \tag{1.40}$$

where $\gamma \equiv \alpha K_T / \rho c_v$ is the dimensionless Grüneisen parameter. Now, we may put (1.32) into (1.28) and obtain the final form of the heat equation:

$$\rho c_v \frac{\partial T}{\partial t} = \nabla \cdot (\boldsymbol{k} \cdot \nabla T) - \rho c_v \boldsymbol{v} \cdot \nabla T - \rho c_v T \gamma \nabla \cdot \boldsymbol{v} + \boldsymbol{\sigma} : \nabla \boldsymbol{v} + H \quad \text{inside } V(t) \setminus \Sigma(t) \, . \tag{1.41}$$

Here the l.h.s. represents local time changes of temperature and the term $-\rho c_v \boldsymbol{v} \cdot \nabla T$ is the advection of heat.

1.3.2 Heat equation in p, T variables

Consider pressure and temperature to be independent variables. Then

$$\rho T \frac{Ds}{Dt} = \rho T \left(\frac{\partial s}{\partial T}\right)_p \frac{DT}{Dt} + \rho T \left(\frac{\partial s}{\partial p}\right)_T \frac{Dp}{Dt} = \rho c_p \frac{DT}{Dt} + \rho \xi \frac{Dp}{Dt} \, , \tag{1.42}$$

where c_p is the isobaric specific heat and $\xi \equiv T\left(\frac{\partial s}{\partial p}\right)_T$. We again need to express ξ by means of measurable quantities. The same procedure as in the section 1.3.1 gives

$$T\, ds = T\left(\frac{\partial s}{\partial T}\right)_p dT + T\left(\frac{\partial s}{\partial p}\right)_T dp = c_p\, dT + \xi\, dp \, , \tag{1.43}$$

$$T\, dS = dU + p\, dV = \left[\left(\frac{\partial U}{\partial T}\right)_p + p\left(\frac{\partial V}{\partial T}\right)_p\right] dT + \left[\left(\frac{\partial U}{\partial p}\right)_T + p\left(\frac{\partial V}{\partial p}\right)_T\right] dp = c_p\, dT + \xi\, dp \, . \tag{1.44}$$

Now (1.43) and (1.44) yield

$$\left(\frac{\partial c_p}{\partial p}\right)_T - \left(\frac{\partial \xi}{\partial T}\right)_p = -\left(\frac{\partial s}{\partial p}\right)_T \tag{1.45}$$

and

$$\left(\frac{\partial c_p}{\partial p}\right)_T - \left(\frac{\partial \xi}{\partial T}\right)_p = \left(\frac{\partial V}{\partial T}\right)_p . \tag{1.46}$$

Hence

$$\xi = -T\left(\frac{\partial V}{\partial T}\right)_p = -TV\alpha = -\frac{\alpha T}{\rho} \tag{1.47}$$

and the final form of the heat equation is

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (\boldsymbol{k} \cdot \nabla T) - \rho c_p \boldsymbol{v} \cdot \nabla T + \alpha T(\frac{\partial p}{\partial t} + \boldsymbol{v} \cdot \nabla p) + \boldsymbol{\sigma} : \nabla \boldsymbol{v} + H . \tag{1.48}$$

The equation of continuity (1.5) yields

$$\nabla \cdot \boldsymbol{v} = -\frac{1}{\rho}\frac{D\rho}{Dt} = -K_T^{-1}\frac{Dp}{Dt} + \alpha \frac{DT}{Dt} , \tag{1.49}$$

and thus the heat equation (1.48) becomes the same as (1.41) with

$$c_p = c_v(1 + \gamma \alpha T) . \tag{1.50}$$

1.3.3 Heat equation in a continuum with dominant hydrostatic pressure

Suppose that there exists a motionless state ($\boldsymbol{v}$=0), characterized by a reference temperature T_0 and a reference density distribution ρ_0. According to the momentum equation (1.10) and the rheological relationship (1.25) it holds

$$\nabla p_0 = \rho_0 \boldsymbol{g}_0 - \rho_0 \boldsymbol{\Omega} \times (\boldsymbol{\Omega} \times \boldsymbol{r}) , \tag{1.51}$$

where $\boldsymbol{g}_0$ is the gravity acceleration due to the gravitational potential of the reference density distribution ρ_0 and the centrifugal potential. [6] Throughout this section we will assume that even in a moving continuum this hydrostatic pressure is much higher than the difference $p - p_0$ and thus we will consider only the hydrostatic pressure dependences.

Assuming the dominance of the hydrostatic pressure we may now put $\partial p/\partial t + \boldsymbol{v} \cdot \nabla p = -v_r \rho g$, with v_r being the radial component of velocity, and $g = |\boldsymbol{g}|$, $\boldsymbol{g} = \boldsymbol{g}_0 - \boldsymbol{\Omega} \times (\boldsymbol{\Omega} \times \boldsymbol{r})$, [7] and obtain thus the usual form of the heat equation

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (\boldsymbol{k} \cdot \nabla T) - \rho c_p \boldsymbol{v} \cdot \nabla T - \rho v_r \alpha T g + \boldsymbol{\sigma} : \nabla \boldsymbol{v} + H . \tag{1.52}$$

[6] In a general case, external sources of the gravity field may be considered by means of a constant part of the tidal potential.

[7] Here we simply suppose that the radial unit vector $\boldsymbol{e}_r \doteq -\boldsymbol{g}/g$.

Interpret now the term $-\rho v_r \alpha T g$. The second thermodynamic law (1.43) for an adiabatic process states

$$\left(\frac{\partial T}{\partial p}\right)_s = -\frac{\xi}{c_p} = \frac{\alpha T}{\rho c_p} \tag{1.53}$$

according to (1.47). Since

$$\left(\frac{\partial T}{\partial p}\right)_s = \left(\frac{\partial T}{\partial r}\right)_s \left(\frac{\partial r}{\partial p}\right)_s = -\frac{1}{\rho g}\left(\frac{\partial T}{\partial r}\right)_s , \tag{1.54}$$

we obtain that the *adiabatic gradient* in the continuum is

$$\left(\frac{\partial T}{\partial r}\right)_s = -\frac{\alpha T g}{c_p} . \tag{1.55}$$

If we add together the radial advection of heat $-\rho c_p v_r \partial T/\partial r$ and the term $-\rho v_r \alpha T g = -\rho c_p v_r \frac{\alpha T g}{c_p}$, we can easily see that a radial motion can locally heat or cool the continuum only in the case when the vertical component of the gradient of temperature is not equal to the adiabatic gradient. This is the reason why the term $\rho v_r \alpha T g$ is called the *adiabatic heating.*

1.3.4 Summary of fundamental equations

The basic equations in the region $V(t) \setminus \Sigma(t)$ are:

Equation of continuity

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = 0 .$$

Equation of continuity of radioactive heat sources

$$\frac{\partial R}{\partial t} + \nabla \cdot (R\boldsymbol{v}) = -\sum_i \rho c_i \frac{Z_i}{\lambda_i} e^{-\frac{t}{\lambda_i}} .$$

Momentum equation

$$\nabla \cdot \boldsymbol{\tau} + \rho \boldsymbol{g} - 2\rho \boldsymbol{\Omega} \times \boldsymbol{v} - \rho \boldsymbol{\Omega} \times (\boldsymbol{\Omega} \times \boldsymbol{r}) = \rho \frac{\partial \boldsymbol{v}}{\partial t} + \rho \boldsymbol{v} \cdot \nabla \boldsymbol{v} .$$

Conservation of moment of momentum

$$\boldsymbol{\tau} = (\boldsymbol{\tau})^T .$$

Rheological relationship

$$\boldsymbol{\tau} = -p\boldsymbol{I} + \boldsymbol{\sigma}(\boldsymbol{v}) , \quad \lim_{\boldsymbol{v}\to 0} \boldsymbol{\sigma}(\boldsymbol{v}) = 0 ,$$

Heat equation

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (\boldsymbol{k} \cdot \nabla T) - \rho c_p \boldsymbol{v} \cdot \nabla T - \rho v_r \alpha T g + \boldsymbol{\sigma} : \nabla \boldsymbol{v} + H \,.$$

Equation of state

$$\rho = \rho(p, T) \,.$$

The basic boundary conditions expressing the laws of conservation (as well as the thermodynamic requirement on continuity of temperature) on an internal interface $\Sigma(t)$ are:

Equation of continuity

$$[\rho(\boldsymbol{v} - \boldsymbol{\nu})]_-^+ \cdot \boldsymbol{n} = 0 \,.$$

Momentum equation

$$[\rho \boldsymbol{v}(\boldsymbol{v} - \boldsymbol{\nu}) - \boldsymbol{\tau}]_-^+ \cdot \boldsymbol{n} = 0 \,.$$

Energy balance

$$[\boldsymbol{k} \cdot \nabla T]_-^+ \cdot \boldsymbol{n} = [\rho \epsilon (\boldsymbol{v} - \boldsymbol{\nu})]_-^+ \cdot \boldsymbol{n} + [\frac{1}{2}\rho(\boldsymbol{v} \cdot \boldsymbol{v})(\boldsymbol{v} - \boldsymbol{\nu})]_-^+ \cdot \boldsymbol{n} - [\boldsymbol{v} \cdot \boldsymbol{\tau}]_-^+ \cdot \boldsymbol{n} \,.$$

Continuation of temperature

$$[T]_-^+ = 0 \,.$$

Moreover, it is necessary to describe a physical nature of the interface Σ. Let us start with properties in the normal direction to the interface. In the Earth, a typical interface can be formed by *the contact boundary* between two different materials with no flow passing through. In geodynamics, such a boundary is frequently called *chemical* to emphasize that the contact is ususally caused by the existence of two regions with chemically distinct properties. In such a case, the equation of continuity is replaced simply by

$$[\boldsymbol{v} - \boldsymbol{\nu}]^+ \cdot \boldsymbol{n} = [\boldsymbol{v} - \boldsymbol{\nu}]^- \cdot \boldsymbol{n} = 0 \quad \Rightarrow \quad [\boldsymbol{v}]_-^+ \cdot \boldsymbol{n} = 0 \tag{1.56}$$

as $[\boldsymbol{\nu}]_-^+ = 0$. The momentum equation thus simplifies to

$$[\boldsymbol{\tau}]_-^+ \cdot \boldsymbol{n} = 0 \tag{1.57}$$

and the energy conservation law comes into the form

$$[\boldsymbol{k} \cdot \nabla T]_-^+ \cdot \boldsymbol{n} = -[(\boldsymbol{v} - (\boldsymbol{v} \cdot \boldsymbol{n})\boldsymbol{n}) \cdot \boldsymbol{\tau}]_-^+ \cdot \boldsymbol{n} \,; \tag{1.58}$$

(here we used both (1.56) and (1.57)). On the other side, if the interface is created by a *phase transition*, its kinetics is a complicated matter controlled by the pressure, the temperature and particle velocities, i.e., $\boldsymbol{\nu} = \boldsymbol{\nu}(p, T, \boldsymbol{v})$ (it is usual to consider simply

$\boldsymbol{\nu} = 0$ in many geodynamical applications). In this case all laws of conservation on the interface must be taken into account in their original form.

To complete the boundary conditions on $\Sigma(t)$, it is also necessary to determine its tangential slip properties. For example, *no slip internal boundary* is defined by the conditions

$$[\boldsymbol{v} - (\boldsymbol{v} \cdot \boldsymbol{n})\boldsymbol{n}]_-^+ = 0\,, \tag{1.59}$$

whereas in the case of *the free-slip internal boundary*

$$\boldsymbol{\tau} \cdot \boldsymbol{n} = ((\boldsymbol{\tau} \cdot \boldsymbol{n}) \cdot \boldsymbol{n})\boldsymbol{n} \tag{1.60}$$

must hold on both sides of the interface $\Sigma(t)$. In the both cases (1.58) simplifies to

$$[\boldsymbol{k} \cdot \nabla T]_-^+ \cdot \boldsymbol{n} = 0\,, \tag{1.61}$$

i.e. in the cases of the no slip or the free slip contact boundary the heat flux passing through the boundary is continuous.

In the case of the contact interface with no slip, (1.56) and (1.59) can be joined into the concise form

$$[\boldsymbol{v}]_-^+ = 0\,, \tag{1.62}$$

which, together with (1.57), represents six independent mechanical conditions. On the other side, the equation (1.60) represents four independent conditions. The consequence of (1.60) is that the momentum equation on $\Sigma(t)$ can be rewritten as follows,

$$[\rho(\boldsymbol{v} \cdot \boldsymbol{n})(\boldsymbol{v} - \boldsymbol{\nu}) \cdot \boldsymbol{n}]_-^+ = [(\boldsymbol{\tau} \cdot \boldsymbol{n}) \cdot \boldsymbol{n}]_-^+ \tag{1.63}$$

and

$$[\rho(\boldsymbol{v} - (\boldsymbol{v} \cdot \boldsymbol{n})\boldsymbol{n})(\boldsymbol{v} - \boldsymbol{\nu}) \cdot \boldsymbol{n}]_-^+ = 0\,. \tag{1.64}$$

Hence, in the case of the contact interface with free-slip, (1.64) is satisfied implicitly, (1.63) reduces to

$$[(\boldsymbol{\tau} \cdot \boldsymbol{n}) \cdot \boldsymbol{n}]_-^+ = 0 \tag{1.65}$$

and the system (1.56), (1.60) and (1.63) again consists of six independent mechanical conditions.

Finally, we need to add the boundary conditions on the surface of the planet. Neglecting all forces due to, e.g., winds, water etc., we may consider the surface to be *the free boundary*, i.e.,

$$\boldsymbol{\tau} \cdot \boldsymbol{n} = 0 \quad \text{on } S(t)\,. \tag{1.66}$$

Note that we consider here that the surface is moving. In fact, this boundary condition defines the topography undulations caused by internal dynamical forces throughout the time evolution. However, it is a complicated problem from the numerical point of view, if one deals with the studied system of partial differential equations in a domain with a moving boundary. This is the reason why the boundary condition (1.66) is sometimes replaced by the *fixed impermeable boundary with the free-slip*, i.e., the condition (1.60) is considered together with the demand

$$\boldsymbol{v} \cdot \boldsymbol{n} = 0 \quad \text{on } S(t) \equiv S_0 \,, \tag{1.67}$$

where S_0 is an a priori chosen fixed surface. One then obtains a force acting just along the normal direction to the surface, which may be interpreted as the linearization of the dynamic force, which could modulate the surface in the case of the free boundary. As to the heat equation, it is well known that the surface temperature is determined by the balance between the energy falling to the surface from the Sun and the energy radiated from the Earth's surface because the internal heat flow, which could break this balance, may be omitted in these considerations. Therefore,

$$T(t) = T_0(t) \quad \text{on } S(t) \tag{1.68}$$

is an independent boundary condition with $T_0(t)$ being a function defined on $S(t)$.

Chapter 2

Thermal conduction

In this chapter we will deal with the equation of heat conduction in the form

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + R \,. \tag{2.1}$$

In geophysics, this form of the heat equation is applicable to problems associated with the heat state of a part of a lithospheric plate. If the reference frame is attached to a lithospheric plate and if we do not take into account such effects like the motion of underground water, motion of hot magma, deformation of the lithospheric plate etc., there is no motion of material relatively to the axes of a reference frame, in which the heat equation is expressed. Interactions of the lithospheric plate with its exterior may be included by means of boundary conditions. We will start with the simplest one-dimensional (1-D) cases that are characterized by only a depth-dependence of a problem. If the physical properties of continuum are constant, then it is possible to find analytical solutions as demonstrated in the next section.

2.1 Analytical solutions of 1-D problems

2.1.1 Homogeneous equation for a finite depth interval

Let us start with the problem how to determine the temperature distribution in a layer of thickness h if the surface temperature $T = T_0$, the bottom temperature $T = T_h$ and the initial temperature distribution in time $t = 0$ is described by a function $\phi(z)$, where z is the depth. We will not take into account any internal heating now. Density, specific heat and thermal conductivity will be constant. This means that (2.1) reduces to

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial z^2} \,, \tag{2.2}$$

where we introduced the thermal diffusivity κ, which is defined by the relation $\kappa = k/\rho c_p$, with the initial condition

$$T(z,0) = \phi(z) \tag{2.3}$$

and the boundary conditions

$$T(0,t) = T_0\,, \quad T(h,t) = T_h\,. \tag{2.4}$$

To satisfy the nonhomogeneous boundary condition, we will write

$$T(z,t) = T_0 + \frac{z}{h}(T_h - T_0) + T'(z,t)\,. \tag{2.5}$$

T' satisfies (2.2) with homogeneous boundary conditions $T'(0,t) = T'(h,t) = 0$ and the initial condition

$$T'(z,0) = \phi'(z) \equiv \phi(z) - T_0 - \frac{z}{h}(T_h - T_0) \tag{2.6}$$

Let us try to find the solution of the problem by means of the separation of variables, i.e.,

$$T'(z,t) = Z(z)X(t)\,. \tag{2.7}$$

Equation (2.2) then yields

$$\frac{1}{\kappa X}\frac{\partial X}{\partial t} = \frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}\,. \tag{2.8}$$

This equation can hold only if both sides are equal to a constant c. Then $X \sim \exp(c\kappa t)$ and, therefore, c must be negative to obtain a convergent solution. Hence, $Z = a\sin\sqrt{|c|}z + b\cos\sqrt{|c|}z$, where a and b are constants. The homogeneous boundary conditions require $b = 0$ and $\sin\sqrt{|c|}h = 0$. This implies that the admissible values of c create the infinite set

$$c_n = -\left(\frac{n\pi}{h}\right)^2\,,\ n = 1,2,3,\ldots \tag{2.9}$$

and the solution T' may be expressed in the form of the series

$$T'(z,t) = \sum_{n=1}^{\infty} a_n \exp\left(-\kappa\left(\frac{n\pi}{h}\right)^2 t\right)\sin\frac{n\pi}{h}z\,. \tag{2.10}$$

The constants a_n can be determined from the initial condition (2.6) as follows

$$\sum_{n=1}^{\infty} a_n \sin\frac{n\pi}{h}z = \phi'(z)\,. \tag{2.11}$$

The l.h.s. of (2.11) represents the Fourier series with the basis functions $\sin\left(\frac{n\pi}{h}z\right)$. Any coefficient a_k may be obtained in a standard way multiplying (2.11) by $\sin\left(\frac{k\pi}{h}z\right)$ and integrating over the depth.

$$a_k = \frac{\int_0^h \sin\left(\frac{k\pi}{h}\xi\right)\phi'(\xi)\,d\xi}{\int_0^h \sin^2\left(\frac{k\pi}{h}\xi\right)\,d\xi} = \frac{2}{h}\int_0^h \sin\left(\frac{k\pi}{h}\xi\right)\phi'(\xi)\,d\xi\,. \tag{2.12}$$

Hence,

$$T'(z,t) = \sum_{n=1}^{\infty} \frac{2}{h} \int_0^h \sin\left(\frac{n\pi}{h}\xi\right) \phi'(\xi) \exp\left(-\kappa \left(\frac{n\pi}{h}\right)^2 t\right) \sin\left(\frac{n\pi}{h}z\right) \, d\xi \,. \tag{2.13}$$

If ϕ is a bounded function, we have for any $t > 0$

$$\left|\sin\left(\frac{n\pi}{h}\xi\right) \phi'(\xi) \exp\left(-\kappa \left(\frac{n\pi}{h}\right)^2 t\right) \sin\left(\frac{n\pi}{h}z\right)\right| \leq \max_{\xi \in <0,h>} |\phi'(\xi)| \exp\left(-\kappa \left(\frac{n\pi}{h}\right)^2 t\right) \to 0 \tag{2.14}$$

if $n \to \infty$. We can thus change the order of summation and integration and write

$$T'(z,t) = \int_0^h \left\{ \sum_{n=1}^{\infty} \frac{2}{h} \sin\left(\frac{n\pi}{h}\xi\right) \sin\left(\frac{n\pi}{h}z\right) \exp\left(-\kappa \left(\frac{n\pi}{h}\right)^2 t\right) \right\} \phi'(\xi) \, d\xi \equiv$$

$$\equiv \int_0^h G(z,\xi,t) \phi'(\xi) \, d\xi \,, \tag{2.15}$$

where $G(z,\xi,t)$ is the *Green function* of the homogeneous problem. Since $\phi'(\xi)$ is given by (2.6), let us try to express $-\int_0^h G(z,\xi,t)[T_0 + \frac{\xi}{h}(T_h - T_0)] \, d\xi$. It holds

$$\int_0^h T_0 \sin\left(\frac{n\pi}{h}\xi\right) \, d\xi = T_0 \frac{h}{n\pi} \left[-\cos\frac{n\pi}{h}\xi\right]_0^h = T_0 \frac{h}{n\pi} \left((-1)^{n+1} + 1\right) \tag{2.16}$$

and

$$\int_0^h (T_h - T_0) \frac{\xi}{h} \sin\left(\frac{n\pi}{h}\xi\right) \, d\xi = \frac{T_h - T_0}{n\pi} \left[-\xi \cos\frac{n\pi}{h}\xi\right]_0^h + \int_0^h \frac{T_h - T_0}{n\pi} \cos\left(\frac{n\pi}{h}\xi\right) \, d\xi =$$

$$= \frac{T_h - T_0}{n\pi} h(-1)^{n+1} \,. \tag{2.17}$$

Therefore,

$$-\int_0^h \sin\left(\frac{n\pi}{h}\xi\right) \left[T_0 + \frac{\xi}{h}(T_h - T_0)\right] \, d\xi = -\frac{h}{n\pi} \left(T_0 + (-1)^{n+1} T_h\right) \tag{2.18}$$

and thus the final expression of T is

$$T(z,t) = T_0 + \frac{z}{h}(T_h - T_0) - \sum_{n=1}^{\infty} \frac{2}{n\pi} \left(T_0 + (-1)^{n+1} T_h\right) \exp\left(-\kappa \left(\frac{n\pi}{h}\right)^2 t\right) \sin\left(\frac{n\pi}{h}z\right) +$$

$$+ \int_0^h G(z,\xi,t) \phi(\xi) \, d\xi \,. \tag{2.19}$$

2.1.2 Equation with heat sources for a finite depth interval

Let us extend the equation (2.2) by the heating term, i.e.,

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial z^2} + Q(z,t)\,, \quad Q(z,t) = R(z,t)/\rho c_p \tag{2.20}$$

and try to find the solution satisfying the initial and boundary conditions (2.3), (2.4). If we write $T = T_1 + T_2$, where T_1 is given by (2.19) and T_2 represents the influence of internal heating, T_2 must satisfy the extended equation (2.20) with homogeneous boundary and initial conditions $T_2(z,0) = T_2(0,t) = T_2(h,t) = 0$. Expand T_2 into the series

$$T_2(z,t) = \sum_{n=1}^{\infty} k_n(t) \sin\left(\frac{n\pi}{h} z\right)\,, \tag{2.21}$$

where we choose $k_n(0) = 0 \ \forall n \geq 1$ to satisfy the initial condition.

Expand analogically heat sources

$$Q(z,t) = \sum_{n=1}^{\infty} q_n(t) \sin\left(\frac{n\pi}{h} z\right)\,; \quad q_n(t) = \frac{2}{h}\int_0^h \sin\left(\frac{n\pi}{h}\xi\right) Q(\xi,t)\,d\xi\,. \tag{2.22}$$

Putting the expansions (2.21) and (2.22) into (2.20) we arrive at the system of decoupled ordinary differential equations

$$\frac{d\,k_n(t)}{d\,t} + \kappa\frac{n^2\pi^2}{h^2} k_n(t) = q_n(t) \ \ \forall n \geq 1\,. \tag{2.23}$$

Solution of (2.23), with the initial condition $k_n = 0$, is given by the convolution of a transfer function u_n with q_n

$$k_n(t) = \int_0^t u_n(t-\tau) q_n(\tau)\,d\tau\,. \tag{2.24}$$

Then

$$u_n(0)q_n(t) + \int_0^t \frac{\partial u_n(t-\tau)}{\partial t} q_n(\tau)\,d\tau + \kappa\frac{n^2\pi^2}{h^2}\int_0^t u_n(t-\tau)q_n(\tau)\,d\tau = q_n(t)\,. \tag{2.25}$$

Choosing the initial value $u_n(0) = 1$ it is clear that u_n must satisfy (2.23) with zero r.h.s. Hence

$$u_n(t) = \exp\left(-\kappa\frac{n^2\pi^2}{h^2} t\right)\,. \tag{2.26}$$

If Q is bounded, we may again rearrange summation and integration and obtain from (2.21), (2.22), (2.24) and (2.26)

$$T_2(z,t) = \int_0^t \left[\int_0^h \left\{\sum_{n=1}^{\infty} \frac{2}{h}\sin\left(\frac{n\pi}{h}\xi\right) \sin\left(\frac{n\pi}{h}z\right) \exp\left(-\kappa\left(\frac{n\pi}{h}\right)^2 (t-\tau)\right)\right\} Q(\xi,\tau)\,d\xi\right] d\tau\,. \tag{2.27}$$

Comparing (2.27) with (2.25) we can see that the influence of internal heating is expressed by means of the same Green function as the influence of the initial condition. The final solution of the problem described by the equations (2.20), (2.3) and (2.4) thus attains a relatively simple form

$$T(z,t) = T_0 + \frac{z}{h}(T_h - T_0) - \sum_{n=1}^{\infty} \frac{2}{n\pi}\left(T_0 + (-1)^{n+1} T_h\right) \exp\left(-\kappa \left(\frac{n\pi}{h}\right)^2 t\right) \sin\left(\frac{n\pi}{h} z\right) +$$

$$+ \int_0^h G(z,\xi,t)\phi(\xi)\, d\xi + \int_0^t \left(\int_0^h G(z,\xi,t-\tau) Q(\xi,\tau)\, d\xi\right) d\tau \,. \tag{2.28}$$

2.1.3 Half-space problems

In the applications concerning the cooling of shallow subsurface parts of the Earth it is advantageous to approximate the Earth simply by a half-space, i.e., to consider the depth $z \in < 0, \infty)$. Such an approximation provides us with the basic physics of the problem if the influence of the lower boundary condition is negligible. In this section, we will first find the Green function for the heat conduction in the whole-space ($z \in (-\infty, \infty)$) and then we will employ it for heat conduction in a half-space.

Choosing $\phi'(\xi) = \delta(\xi - a)$ (δ is the Dirac delta-function) in (2.15), we get $T'(z,t) = G(z,a,t)$. This is the reason why we may find the Green function for whole-space problems directly as the solution of the problem

$$\frac{\partial G}{\partial t} = \kappa \frac{\partial^2 G}{\partial z^2}\,, \quad z \in (-\infty, \infty) \tag{2.29}$$

with the initial condition

$$G(z,\xi,0) = \delta(z - \xi)\,. \tag{2.30}$$

We will be employing the Fourier transform

$$\hat{G}(\lambda,\xi,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} G(z,\xi,t) e^{-i\lambda z}\, dz\,, \tag{2.31}$$

where λ is the wavenumber. The inverse Fourier transform is given by the formula

$$G(z,\xi,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{G}(\lambda,\xi,t) e^{i\lambda z}\, d\lambda\,. \tag{2.32}$$

Application of the Fourier transform to (2.29), (2.30) yields

$$\frac{\partial \hat{G}}{\partial t} = -\kappa \lambda^2 \hat{G}\,, \quad \hat{G}(\lambda,\xi,0) = \frac{1}{\sqrt{2\pi}} e^{-i\lambda\xi} \tag{2.33}$$

and the solution of this problem is

$$\hat{G}(\lambda,\xi,t) = \frac{1}{\sqrt{2\pi}} e^{-(i\lambda\xi + \lambda^2 \kappa t)}\,. \tag{2.34}$$

To obtain $G(z,\xi,t)$ we must apply the inverse transform (2.32) to (2.34). It holds

$$G(z,\xi,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-\lambda(i\xi+\lambda\kappa t - iz)}\,d\lambda = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-(\sqrt{\kappa t}\lambda + \frac{i}{2}\frac{(\xi-z)}{\sqrt{\kappa t}})^2}\, e^{-\frac{(\xi-z)^2}{4\kappa t}}\,d\lambda =$$

$$= \frac{1}{2\pi}e^{-\frac{(\xi-z)^2}{4\kappa t}}\int_{-\infty+\frac{i}{2}\frac{(\xi-z)}{\sqrt{\kappa t}}}^{\infty+\frac{i}{2}\frac{(\xi-z)}{\sqrt{\kappa t}}} e^{-u^2}\frac{du}{\sqrt{\kappa t}} = \frac{1}{2\pi}e^{-\frac{(\xi-z)^2}{4\kappa t}}\int_{-\infty}^{\infty} e^{-u^2}\frac{du}{\sqrt{\kappa t}} = \frac{1}{2\sqrt{\pi\kappa t}}e^{-\frac{(\xi-z)^2}{4\kappa t}}\,, \quad (2.35)$$

where we have used the residuum theorem to change the integration path and the formula $\int_{-\infty}^{\infty} e^{-u^2}\,du = \sqrt{\pi}$.

A general formulation of the half-space problem is

$$\frac{\partial T}{\partial t} = \kappa\frac{\partial^2 T}{\partial z^2} + Q\,, \quad z \in <0,\infty)\,, \quad (2.36)$$

$$T(0,t) = T_0\,, \quad (2.37)$$

$$T(z,0) = T_0 + \phi(z)\,. \quad (2.38)$$

Writing the solution in the form $T = T_0 + T_1$ we have

$$\frac{\partial T_1}{\partial t} = \kappa\frac{\partial^2 T_1}{\partial z^2} + Q\,, \quad z \in <0,\infty)\,, \quad (2.39)$$

$$T_1(0,t) = 0\,, \quad (2.40)$$

$$T_1(z,0) = \phi(z)\,. \quad (2.41)$$

Let us formally define $\phi(z) = -\phi(-z)$ and $Q(z,t) = -Q(-z,t)$ for $z < 0$. Then we may solve the equation (2.39) with the initial condition (2.41) on the whole space. Because of the symmetry of the continuation of the initial condition as well as heat sources, it is clear that the condition (2.40) is satisfied, too. We have thus arrived at the solution of the system (2.36)–(2.38) as follows

$$T = T_0 + \frac{1}{2\sqrt{\pi\kappa t}}\int_0^{\infty}\left[e^{-\frac{(z-\xi)^2}{4\kappa t}} - e^{-\frac{(z+\xi)^2}{4\kappa t}}\right]\phi(\xi)\,d\xi +$$

$$+ \frac{1}{2\sqrt{\pi\kappa}}\int_0^t\int_0^{\infty}\left[e^{-\frac{(z-\xi)^2}{4\kappa(t-\tau)}} - e^{-\frac{(z+\xi)^2}{4\kappa(t-\tau)}}\right]\frac{Q(\xi,\tau)}{\sqrt{t-\tau}}\,d\tau d\xi\,. \quad (2.42)$$

If $\phi(\xi) = \phi_0 = \text{const.}$, we may write

$$\frac{1}{2\sqrt{\pi\kappa t}}\int_0^{\infty}\left[e^{-\frac{(z-\xi)^2}{4\kappa t}} - e^{-\frac{(z+\xi)^2}{4\kappa t}}\right]\phi(\xi)\,d\xi = \frac{\phi_0}{2\sqrt{\pi\kappa t}}\int_0^{2z} e^{-\frac{(z-\xi)^2}{4\kappa t}}\,d\xi =$$

$$= \frac{\phi_0}{\sqrt{\pi}}\int_{-\frac{z}{2\sqrt{\kappa t}}}^{\frac{z}{2\sqrt{\kappa t}}} e^{-u^2}\,du = \phi_0\frac{2}{\sqrt{\pi}}\int_0^{\frac{z}{2\sqrt{\kappa t}}} e^{-u^2}\,du \equiv \phi_0\,\mathrm{erf}\left(\frac{z}{2\sqrt{\kappa t}}\right)\,, \quad (2.43)$$

where the function $\mathrm{erf}(x)$ is defined by the relation

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-u^2}\,du\,. \quad (2.44)$$

If, moreover, distribution of heat sources does not depend on the depth z, i.e., $Q(z,t) = Q_0(t)$, we may write the final formula in the form

$$T = T_0 + \phi_0 \,\mathrm{erf}\left(\frac{z}{2\sqrt{\kappa t}}\right) + \int_0^t Q_0(\tau)\,\mathrm{erf}\left(\frac{z}{2\sqrt{\kappa(t-\tau)}}\right) d\tau \,. \tag{2.45}$$

If T_0 is not a constant but a function of time, $T_0 = T_0(t)$, (2.42) does not satisfy the heat equation (2.36) since $\partial T_0/\partial t \neq 0$. It is necessary to add the term $-\int_0^t \frac{\partial T_0}{\partial t}(\tau)\,\mathrm{erf}(\frac{z}{2\sqrt{\kappa(t-\tau)}})\,d\tau$ to the r.h.s. of (2.42). The special case is when we deal with the influence of time-periodic changes of the boundary condition, i.e., with the system

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial z^2}\,, \quad z \in < 0, \infty)\,, \tag{2.46}$$

$$T(0,t) = T_0 + T_c e^{i\omega t}\,, \quad t \in (-\infty, \infty)\,. \tag{2.47}$$

When we try to find the solution in the form $T = T_0 + T_1(z)e^{i\omega t}$, it is easy to get

$$T = T_0 + T_c e^{-\sqrt{\frac{\omega}{2\kappa}}z} e^{i\left(\omega t - \sqrt{\frac{\omega}{2\kappa}}z\right)}\,. \tag{2.48}$$

Basic properties of a heat wave generated by time-periodic changes of the surface temperature are thus described by means of $\sqrt{\frac{\omega}{2\kappa}}$: $\sqrt{\frac{2\kappa}{\omega}}$ is the characteristic depth of penetration and $\sqrt{\frac{\omega}{2\kappa}}z$ is the phase shift of the wave.

2.1.4 Cooling of the oceanic lithosphere

Half-space model

The mid-oceanic ridges are the locations where mantle material of temperature T_m flows upward creating thus new oceanic lithosphere. If we suppose that the lithosphere after its creation moves only horizontally and if we take into account only vertical conduction of heat (neglecting thus conduction in horizontal direction), the temperature of the cooling lithosphere is described by the system (2.36)–(2.38), where t is the age of the lithosphere, T_0 is the temperature of the bottom of the ocean and $\phi(z) = T_m - T_0$. Heat sources do not play a substantial role in the oceanic lithosphere and, therefore, will be neglected, too. According to (2.45), the model is given by the relation

$$T = T_0 + (T_m - T_0)\,\mathrm{erf}\left(\frac{z}{2\sqrt{\kappa t}}\right)\,. \tag{2.49}$$

The averaged oceanic floor is not flat but the depth of the ocean rises with increasing age. Suppose that, in the first approximation, the lithosphere is in an isostatic equilibrium, i.e., the excess of mass due to the lower depth of the oceanic floor is compensated by the lower density caused by higher temperature of the lithosphere. If ρ_m is the mass density of the lithosphere under the temperature T_m, ρ_w is density of water and $b(t)$ is the difference between the depth of the ocean of the age t and the depth of the mid-ocean ridge, the equilibrium may be expressed as follows

$$(\rho_m - \rho_w)b = \int_0^\infty \rho_m \alpha (T_m - T)\, dz\,, \tag{2.50}$$

i.e.,

$$b = \frac{\alpha \rho_m (T_m - T_0)}{\rho_m - \rho_w} \int_0^\infty \mathrm{erfc}\left(\frac{z}{2\sqrt{\kappa t}}\right) dz\,, \tag{2.51}$$

where

$$\mathrm{erfc}(x) = 1 - \mathrm{erf}(x)\,. \tag{2.52}$$

The integral in (2.51) may be computed per partes

$$\int_0^\infty 1\, \mathrm{erfc}\left(\frac{z}{2\sqrt{\kappa t}}\right) dz = \left[z\, \mathrm{erfc}\left(\frac{z}{2\sqrt{\kappa t}}\right)\right]_0^\infty + \frac{1}{\sqrt{\pi \kappa t}} \int_0^\infty z e^{-\left(\frac{z}{2\sqrt{\kappa t}}\right)^2} dz =$$

$$= \frac{2\sqrt{\kappa t}}{\sqrt{\pi}} \int_0^\infty e^{-y}\, dy = \frac{2\sqrt{\kappa t}}{\sqrt{\pi}} \tag{2.53}$$

and, hence,

$$b = \frac{\alpha \rho_m (T_m - T_0)}{\rho_m - \rho_w} \frac{2\sqrt{\kappa t}}{\sqrt{\pi}}\,. \tag{2.54}$$

In this model, the depth of the ocean is increasing with the square root of the age of the oceanic floor.

The surface heat flow is

$$q_s = k \left.\frac{\partial T}{\partial z}\right|_{z=0} = k \frac{(T_m - T_0)}{\sqrt{\kappa \pi t}}\,. \tag{2.55}$$

The model thus suggests that the heat flow should diverge ($q \sim 1/\sqrt{t}$) for $t \to 0$. This functional dependence was confirmed by measurements. On the other side, the heat flow should disappear for $t \to \infty$. However, observations in old oceanic basins give approximately constant value for $t > 100$ My. The reason is that the lithosphere is a plate of finite thickness and not an infinite half-space. The influence of the temperature at the bottom of the lithosphere, which is kept more or less constant by mantle processes, is thus not negligible and becomes even dominant for very old lithosphere since it generates constant contribution $k\frac{T_m - T_0}{h}$ to the total heat flow (h is the thickness of the lithosphere). Better approximation is, therefore, plate model that will be described below.

Plate model

As mentioned above, the plate model is characterized by the condition $T = T_m$ at the depth $z = h$. According to (2.19) the temperature distribution is

$$T(z,t) = T_0 + \frac{z}{h}(T_m - T_0) - \sum_{n=1}^{\infty} \frac{2}{n\pi}\left(T_0 + (-1)^{n+1}T_m\right)\exp\left(-\kappa\left(\frac{n\pi}{h}\right)^2 t\right)\sin\left(\frac{n\pi}{h}z\right) +$$

$$+ \int_0^h G(z,\xi,t)T_m\, d\xi =$$

$$= T_0 + \frac{z}{h}(T_m - T_0) + \sum_{n=1}^{\infty} \frac{2}{n\pi}(T_m - T_0)\exp\left(-\kappa\left(\frac{n\pi}{h}\right)^2 t\right)\sin\left(\frac{n\pi}{h}z\right) . \qquad (2.56)$$

The surface heat flow of the plate model can now be simply expressed as follows

$$q_s = k\frac{T_m - T_0}{h} + k\sum_{n=1}^{\infty} \frac{2}{h}(T_m - T_0)\exp\left(-\kappa\left(\frac{n\pi}{h}\right)^2 t\right) . \qquad (2.57)$$

Similarly, the increase of the depth of the sea-floor is

$$b = \frac{\alpha\rho_m}{\rho_m - \rho_w}\int_0^h (T_m - T)\, dz =$$

$$= \frac{\alpha\rho_m(T_m - T_0)}{\rho_m - \rho_w}\left[\frac{h}{2} + \sum_{n=1}^{\infty} \frac{2h}{(n\pi)^2}((-1)^n - 1)\exp\left(-\kappa\left(\frac{n\pi}{h}\right)^2 t\right)\right] .$$

2.2 Downward heat flow continuation

In this section we will deal with the evaluation of the subsurface temperature and heat flow from their surface values. In the first approximation, we may neglect changes in time and consider the temperature field to be steady-state. This means that the fundamental equation of heat conduction is reduced to

$$\nabla \cdot (k\nabla T) + R = 0 . \qquad (2.58)$$

Throughout the whole section we will assume that the thermal conductivity k depends only on the depth z. However, we will distinguish two cases: (i) fully one-dimensional (1-D) problem, where temperature is only a function of depth, too; (ii) three-dimensional (3-D) problem, where temperature may change also in horizontal directions.

2.2.1 1-D problem

Since the horizontal component of ∇T is equal to zero in this approximation, the equation (2.58) is simple relation

$$\frac{d}{dz}\left(k(z)\frac{dT(z)}{dz}\right) + R(z) = 0\,. \tag{2.59}$$

Denoting the magnitude of the upward heat flow by q, we may write

$$q(z_2) - q(z_1) = -\int_{z_1}^{z_2} R(z)\,dz \tag{2.60}$$

and

$$T(z_2) - T(z_1) = \int_{z_1}^{z_2} \frac{q(z)}{k(z)}\,dz = q(z_1)\int_{z_1}^{z_2} \frac{dz}{k(z)} - \int_{z_1}^{z_2} \frac{1}{k(z)}\left(\int_{z_1}^{z} R(\xi)\,d\xi\right)\,dz\,. \tag{2.61}$$

Introducing the vector consisting of temperature and heat flow, (2.60) and (2.61) may be rewritten as follows

$$\begin{pmatrix} T \\ q \end{pmatrix}_{z=z_2} = \begin{pmatrix} 1 & \int_{z_1}^{z_2}\frac{dz}{k(z)} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} T \\ q \end{pmatrix}_{z=z_1} - \begin{pmatrix} \int_{z_1}^{z_2}\frac{1}{k(z)}\left(\int_{z_1}^{z} R(\xi)\,d\xi\right)\,dz \\ \int_{z_1}^{z_2} R(z)\,dz \end{pmatrix}\,. \tag{2.62}$$

This expression relates temperature and heat flow in two arbitrary depths. For example, let $z = z_0$ denote the Earth's surface. We can thus easily compute temperature and heat flow in any depth if we know their surface magnitudes. A special case is a layered model which consists of layers of constant thermal conductivity and heat source. Denoting z_{i-1} and z_i the top and the bottom of the i-th layer, respectively, we may write the following matrix scheme

$$\begin{pmatrix} T \\ q \end{pmatrix}_{z=z_n} = M_n(M_{n-1}(...(M_2(M_1\begin{pmatrix} T \\ q \end{pmatrix}_{z_0} - S_1) - S_2)...) - S_{n-1}) - S_n\,,$$

$$M_i = \begin{pmatrix} 1 & \frac{h_i}{k_i} \\ 0 & 1 \end{pmatrix}\,, \quad S_i = \begin{pmatrix} \frac{h_i^2}{2k_i} \\ h_i \end{pmatrix} R_i\,, \tag{2.63}$$

where h_i is the thickness of the i-th layer, k_i is its thermal conductivity and R_i represents the heat source located in the layer.

2.2.2 3-D problem

Throughout the whole section, we will suppose that we are dealing with anomalies only, i.e., the surface temperature, the surface heat flow as well as the subsurface heat sources are square integrable over the horizontal plane E_2. This means that we do not take into account a background temperature and heat sources distribution yielding, e.g., constant heat flow. We consider the equation

$$\frac{\partial}{\partial z}\left(k(z)\frac{\partial T(x,y,z)}{\partial z}\right) + k(z)\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) T(x,y,z) + R(x,y,z) = 0\,, \tag{2.64}$$

where x and y are horizontal coordinates. Now we will employ the Fourier transform over x and y

$$\hat{T}(\boldsymbol{\lambda}, z) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} T(\boldsymbol{r}, z)\exp\left(-i\boldsymbol{\lambda}\cdot\boldsymbol{r}\right) dx\, dy\ , \tag{2.65}$$

where $\boldsymbol{\lambda}$ is the wavenumber vector and $\boldsymbol{r} = (x, y)$, and obtain

$$\frac{\partial}{\partial z}\left(k(z)\frac{\partial \hat{T}}{\partial z}\right) - k(z)\lambda^2\hat{T} + \hat{R}(z) = 0\,. \tag{2.66}$$

In the case of a layered model, the equation in the i-th layer is

$$\frac{\partial^2\hat{T}}{\partial z^2} - \lambda^2\hat{T} = -\frac{\hat{R}_i}{k_i}\,. \tag{2.67}$$

The solution is

$$\hat{T} = A\cosh\lambda(z - z_{i-1}) + B\sinh\lambda(z - z_{i-1}) + \frac{\hat{R}_i}{k_i\lambda^2}$$

$$A = \hat{T}(z_{i-1}) - \frac{\hat{R}_i}{k_i\lambda^2}\,, \quad B = \frac{\hat{q}_z(z_{i-1})}{k_i\lambda}\,, \quad \hat{q}_z = k\frac{\partial\hat{T}}{\partial z}\,. \tag{2.68}$$

This means that

$$\hat{T}(z_i) = \hat{T}(z_{i-1})\cosh\lambda h_i + \hat{q}_z(z_{i-1})\frac{\sinh\lambda h_i}{k_i\lambda} - \frac{\hat{R}_i}{k_i\lambda^2}(\cosh\lambda h_i - 1)\,,$$

$$\hat{q}_z(z_i) = \hat{T}(z_{i-1})k_i\lambda\sinh\lambda h_i + \hat{q}_z(z_{i-1})\cosh\lambda h_i - \frac{\hat{R}_i}{\lambda}(\sinh\lambda h_i)\,. \tag{2.69}$$

Hence, we may again use the matrix scheme (2.63) with

$$M_i = \begin{pmatrix} \cosh\lambda h_i & (\lambda k_i)^{-1}\sinh\lambda h_i \\ \lambda k_i\sinh\lambda h_i & \cosh\lambda h_i \end{pmatrix}\,, \quad S_i = \begin{pmatrix} (k_i\lambda^2)^{-1}(\cosh\lambda h_i - 1) \\ \lambda^{-1}\sinh\lambda h_i \end{pmatrix}\hat{R}_i\,. \tag{2.70}$$

Formally,

$$\begin{pmatrix} \hat{T} \\ \hat{q}_z \end{pmatrix}_{z=z_n} = A\begin{pmatrix} \hat{T} \\ \hat{q}_z \end{pmatrix}_{z=z_0} + B\,,$$

$$A = M_n M_{n-1}...M_1\,, \quad B = -\sum_{i=1}^{n-1} M_n M_{n-1}...M_{i+1}S_i - S_n \tag{2.71}$$

or, inversely,

$$\begin{pmatrix} \hat{T} \\ \hat{q}_z \end{pmatrix}_{z=z_0} = A^{-1}\begin{pmatrix} \hat{T} \\ \hat{q}_z \end{pmatrix}_{z=z_n} - A^{-1}B\,,$$

$$A^{-1} = M_1^{-1}M_2^{-1}...M_n^{-1}\,, \quad A^{-1}B = -\sum_{i=1}^{n} M_1^{-1}M_2^{-1}...M_i^{-1}S_i\,. \tag{2.72}$$

Regularization of the 3-D downward heat flow continuation

It is clear that A exponentially diverges if $\lambda \to \infty$. Therefore, we must choose a regularization which suppresses this amplification. There are two basic ways of doing this: either to filter data (surface values) in the short-wavelength domain or to confine ourselves to a certain set of admissible models of subsurface values of heat flow and/or temperature and to seek the result of the downward continuation only from this set.

We will demonstrate here the second possibility. In order to simplify the problem, let us fix the surface boundary condition $\hat{T} = 0$. Then

$$\hat{q}_z(z_n) = A_{22}\hat{q}_z(z_0) + B_2 \tag{2.73}$$

and the subsurface heat flow is now only a function of the surface heat flow and heat sources, i.e. (2.73) is an analogy of (2.60). Let us define a set $\mathcal{D}$ of admissible subsurface heat flows symbolically as

$$\mathcal{D} = \{\hat{q}_z(z_n); \hat{q}_z(z_n) \text{ is “good” from the physical point of view}\} .$$

If we now consider only $\hat{q} \in \mathcal{D}$, we may define the *cost functional* F, which expresses a compatibility of $\hat{q}_z$ with the surface heat flow data $\hat{q}_0$:

$$F(\hat{q}_z) = ||\hat{q}_0 - A_{22}^{-1}(\hat{q}_z - B_2)||^2_{L^2(E_2)} , \tag{2.74}$$

where $|| \; ||_{L^2(E_2)}$ is the norm in the space of quadratically integrable functions over the plane E_2 formed by the wavenumber vectors $\boldsymbol{\lambda}$. The term $A_{22}^{-1}B_2$ does not diverge and thus it can be added to $\hat{q}_0$ without any difficulty. The heat flow $\hat{q}_0 + A_{22}B_2$ then represents data which should be interpreted by a heat flow in the depth z_n. The crucial point is that $A_{22}^{-1} \le 1$ and $A_{22}^{-1} \sim \exp(-\lambda(z_n - z_0))$ if $\lambda \to \infty$. Hence, the definition (2.74) has a good sense for any $\mathcal{D}$ bounded in $L^2(E_2)$. The term $A_{22}^{-1}\hat{q}_z$ represents an operator acting to $\hat{q}_z$. From this point of view, the operator A_{22}^{-1} is linear, continuous and injective on $L^2(E_2)$. Therefore, if $\mathcal{D}$ is non-empty, closed, bounded and convex set, then one and only one minimum of F on $\mathcal{D}$ exists. This is the reason why it is natural to replace direct downward heat flow continuation by seeking for the minimum of F on $\mathcal{D}$.

The choice of $\mathcal{D}$ must be made with care. For example, the definition

$$\mathcal{D}_1 = \left\{\hat{q}_z; ||\hat{q}_z||_{L^2(E_2)} \le c, c > 0 \text{ is a given constant}\right\} \tag{2.75}$$

ensures the existence of a unique minimum but the minimum need not be stable as $\hat{q}_z \in \mathcal{D}_1$ need not be small at high wavenumbers. This obstacle can be overcome by constraining the derivatives. Let us define

$$\mathcal{D}_2 = \left\{\hat{q}_z; ||q_z||_{W^{1,2}(E_2)} \le d, d > 0 \text{ is a given constant}\right\} , \tag{2.76}$$

where the norm of a function from Sobolev's space $W^{1,2}(E_2)$ is

$$||q_z||^2_{W^{1,2}(E_2)} = \int_{E_2} q_z^2 \, d\boldsymbol{r} + \int_{E_2} |\nabla q_z|^2 \, d\boldsymbol{r} =$$

$$= \int_{E_2} |\hat{q}_z|^2 \, d\boldsymbol{\lambda} + \int_{E_2} |\widehat{\nabla q_z}|^2 \, d\boldsymbol{\lambda} = \int_{E_2} (1 + \lambda^2) |\hat{q}_z|^2 \, d\boldsymbol{\lambda} \,. \tag{2.77}$$

Hence, all $\hat{q}_z \in \mathcal{D}_2$ are "almost the same" in the domain of high wave number, for they tend to zero if $\lambda \to \infty$, thus yielding the stability of the problem.

Chapter 3

Thermal convection

In this chapter we will take again into account the heat transfer associated with a motion of mass. We will first reformulate the fundamental laws of conservation (see the section 1.3.4) into a form applicable to convection in the Earth and introduce dimensionless quantities. Then we will show the basic characteristics of the Earth's thermal convection from the view of the theory of nonlinear dynamical systems.

3.1 Approximations of the fundamental equations

3.1.1 The Boussinesq approximation of the laws of conservation

The idea of the Boussinesq approximation consists in the linearization of the basic laws of conservation near a reference hydrostatic state, when $\boldsymbol{v} = 0$. If the rheological relationship is in the form

$$\boldsymbol{\tau} = -p\boldsymbol{I} + \boldsymbol{\sigma}(\boldsymbol{v})\,, \quad \lim_{\boldsymbol{v}\to 0} \boldsymbol{\sigma}(\boldsymbol{v}) = 0\,, \tag{3.1}$$

the pressure p_0 and density ρ_0, which characterize (together with temperature T_0) the reference state, are related by the equation

$$\nabla p_0 = \rho_0 \boldsymbol{g}_0 - \rho_0 \boldsymbol{\Omega} \times (\boldsymbol{\Omega} \times \boldsymbol{r})\,. \tag{3.2}$$

If we neglect density changes caused by the pressure deviations $\Pi = p - p_0$, we may linearize the state equation with respect to the temperature deviations $T - T_0$ and write

$$\rho = \rho_0(1 - \alpha(T - T_0))\,, \tag{3.3}$$

where α is the thermal expansion coefficient. This approximation means that the influence of hydrostatic pressure (as well as temperature T_0) on density is hidden into a spatial dependence of the reference density ρ_0.

The reference density ρ_0 is assumed to be a time-independent function. Considering only the largest term in the equation of continuity, i.e. neglecting thermal expansion, we arrive at the simplified equation

$$\nabla \cdot (\rho_0 \boldsymbol{v}) = 0 \,. \tag{3.4}$$

After putting (3.1)–(3.3) into the momentum equation we get

$$-\nabla \Pi + \nabla \cdot \boldsymbol{\sigma} - \rho_0 \alpha (T - T_0) \boldsymbol{g}_\circ + \rho_0 (\boldsymbol{g} - \boldsymbol{g}_\circ) = \rho_0 \left(\frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v} \cdot \nabla \boldsymbol{v} \right) \,, \tag{3.5}$$

where we neglected the quadratic term $-\rho_0 \alpha (T - T_0)(\boldsymbol{g} - \boldsymbol{g}_\circ)$, the Coriolis force and the thermal expansion on the right hand side, i.e., the changes of the inertial force due to thermal expansion. Note that the deviation of the gravity acceleration $\boldsymbol{g} - \boldsymbol{g}_\circ$ is due to the selfgravitation of the Earth. Usually the magnitude of this term is about one order lower than that of the buoyancy term $-\rho_0 \alpha (T - T_0) \boldsymbol{g}_\circ$, therefore, it does not influence substantially the basic physics of the thermal convection. This is the reason why we will omit the selfgravitation term throughout the rest of this chapter. The linearization of the heat equation consists in replacing ρ by ρ_0, i.e.

$$\rho_0 c_p \frac{\partial T}{\partial t} = \nabla \cdot (\boldsymbol{k} \cdot \nabla T) - \rho_0 c_p \boldsymbol{v} \cdot \nabla T - \rho_0 v_r \alpha T g_0 + \boldsymbol{\sigma} : \nabla \boldsymbol{v} + R + H \,. \tag{3.6}$$

The system (3.4)–(3.6) is referred to as the *compressible extended Boussinesq approximation* of the basic laws of conservation. If we neglect compressibility, i.e., if we replace (3.4) by the equation $\nabla \cdot \boldsymbol{v} = 0$, the obtained system of equations is called *(incompressible) extended Boussinesq approximation.*

The *classical Boussinesq approximation* represents a further substantial simplification of the studied system of equations: The reference density ρ_0, the reference gravity acceleration $\boldsymbol{g}_0$, the thermal expansion coefficient α, the isobaric specific heat c_p, the thermal conductivity k are constant; R as well as H are spatially constant (they may be time-dependent), and the above mentioned system is applied to the Newtonian fluid

$$\boldsymbol{\sigma} = \eta (\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T) \tag{3.7}$$

with constant dynamic viscosity η. Moreover, both dissipation $\boldsymbol{\sigma} : \nabla \boldsymbol{v}$ and adiabatic heating $-\rho_0 v_r \alpha T g_0$ are not taken into account. We thus get the system

$$\nabla \cdot \boldsymbol{v} = 0 \,, \tag{3.8}$$

$$-\nabla \Pi + \eta \nabla^2 \boldsymbol{v} - \rho_0 \alpha (T - T_0) \boldsymbol{g}_\circ = \rho_0 \left(\frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v} \cdot \nabla \boldsymbol{v} \right) \,, \tag{3.9}$$

$$\frac{\partial T}{\partial t} = \kappa \nabla^2 T - \boldsymbol{v} \cdot \nabla T + \frac{Q}{\rho_0 c_p} \,, \tag{3.10}$$

where $Q \equiv R + H$.

3.1.2 Boundary conditions

There are several possibilities how to choose the boundary conditions. If the moving continuum is in contact with a solid body, we must fulfill the condition

$$\boldsymbol{v} = 0 \tag{3.11}$$

to avoid infinite stresses on such an interface. This kind of condition is applicable for the convection modelling in the core both on the inner core boundary and on the core-mantle boundary. As to the thermal convection in the mantle, it may be used for the asthenosphere-lithosphere boundary in some applications.

If the lithosphere is incorporated into modelling, we naturally get no-stress condition on the surface:

$$\boldsymbol{\tau} \cdot \boldsymbol{n} = 0\,. \tag{3.12}$$

The problem is that in such a case there is a mass flux through the boundary, which means that the surface is not fixed during time evolution. The problem must then be solved in a domain with changing boundary. Instead, it is possible to employ the combined boundary conditions in the form

$$\boldsymbol{v} \cdot \boldsymbol{n} = 0\,, \tag{3.13}$$

$$\boldsymbol{\tau} \cdot \boldsymbol{n} - ((\boldsymbol{\tau} \cdot \boldsymbol{n}) \cdot \boldsymbol{n})\boldsymbol{n} = 0\,. \tag{3.14}$$

In this case, the normal component of the surface traction $(\boldsymbol{\tau} \cdot \boldsymbol{n}) \cdot \boldsymbol{n}$ need not be zero. The usual procedure is to interpret it like a force keeping nonzero dynamic topography undulations

$$h = -(\boldsymbol{\tau} \cdot \boldsymbol{n}) \cdot \boldsymbol{n}/\rho_s g_s\,, \tag{3.15}$$

where the index s denotes the surface value of a corresponding quantity. The same conditions may be applied to the core-mantle boundary (CMB). However, ρ_s must be replaced by the density jump between the core and the mantle.

In principal, there are two possibilities how to choose a boundary condition for temperature: either to prescribe directly its magnitude (the Dirichlet condition) or to keep the value of heat flow passing through the boundary (the Neumann condition). For example,

$$T = T_s \qquad \text{at the surface}\,, \tag{3.16}$$

$$T = T_b \qquad \text{at the CMB}\,, \tag{3.17}$$

or, respectively

$$k\nabla T \cdot \boldsymbol{n} = q_b \tag{3.18}$$

on a part of the boundary.

3.1.3 Reference temperature

We have not specified the reference temperature distribution T_0 yet. In geothermics, it is usual to adopt a 1-D model of temperature growth in the lithosphere, which may, e.g., correspond with a depth-dependence of the half-space or plate model of the cooling of the lithosphere for a chosen reference age. The extension into the asthenosphere and deeper parts of the mantle is then carried out by means of the estimations of the magnitude of the adiabatic gradient, i.e., it is assumed that the mantle is adiabatic from the bottom of the lithosphere downwards to the top of the D″-layer. In other words, this assumption means that the only boundary layers, where heat conduction plays an important role, are the lithosphere and D″-layer. Since the temperature at the CMB may be estimated from melting experiments with iron, we can also obtain estimations of temperature jump between the top of D″ and the CMB. It is clear that such an approach is rather questionable, because the assumption of adiabaticity need not be valid in and near the transition zone. For example, if the interface between the lower and the upper mantle is at least partly impermeable for mass flow, heat conduction may be the dominant mechanism of heat transfer through this boundary, which contradicts the assumption of adiabaticity.

However, in numerical modelling of thermal convection it is convenient to identify T_0 with the solution of the conduction problem

$$\rho_0 c_p \frac{\partial T_0}{\partial t} = \nabla \cdot (\boldsymbol{k} \cdot \nabla T_0) + R + H \,, \tag{3.19}$$

with corresponding boundary conditions, say (3.16), (3.17). In most of the applications, neither heat sources nor boundary conditions for T_0 are time-dependent, T_0 thus does not depend on time, and the l.h.s. of (3.19) is zero.

The temperature deviation $\Theta \equiv T - T_0$ satisfies

$$\rho_0 c_p \frac{\partial \Theta}{\partial t} = \nabla \cdot (\boldsymbol{k} \cdot \nabla \Theta) - \rho_0 c_p \boldsymbol{v} \cdot \nabla \Theta - \rho_0 v_r \alpha \Theta g_0 - \rho_0 c_p \boldsymbol{v} \cdot \nabla T_0 - \rho_0 v_r \alpha T_0 g_0 + \boldsymbol{\sigma} : \nabla \boldsymbol{v} \tag{3.20}$$

and zero boundary conditions. This is the reason why the role of the source that can generate a nonzero solution of (3.20) is played only by the velocity $\boldsymbol{v}$ of continuum. Since we assume zero r.h.s. of the boundary conditions for velocity (see (3.11)–(3.14)), the only source term in the momentum equation (3.5) is the buoyancy term $-\rho_0 \alpha \Theta \boldsymbol{g}_\circ$. Owing to our assumption $lim_{\boldsymbol{v}\to 0} \boldsymbol{\sigma}(\boldsymbol{v}) = 0$, we may conclude that the studied system yields the trivial solution $\boldsymbol{v} = 0, \Theta = 0, \Pi = 0$, which will be called the *conduction solution* henceforth.

However, the system of equations (3.4), (3.5), (3.20) is nonlinear because of the existence of the terms $\rho_0 \boldsymbol{v} \cdot \nabla \boldsymbol{v}$, $\rho_0 c_p \boldsymbol{v} \cdot \nabla \Theta$, $\rho_0 v_r \alpha \Theta g_0$ and $\boldsymbol{\sigma} : \nabla \boldsymbol{v}$ (nonlinear rheology and/or temperature dependent heat conductivity can represent further nonlinearities). The terms $-\rho_0 c_p \boldsymbol{v} \cdot \nabla T_0 - \rho_0 v_r \alpha T_0 g_0$ in (3.20) can, therefore, be able to keep convection alive. The conditions, when the conduction solution is not stable and convection appears after a fluctuation from the conduction solution will be studied studied for a concrete example in Section ???.

3.1.4 Decomposition into poloidal and toroidal flow components

In this section we will assume that velocity satisfies the equation of continuity in the form $\nabla \cdot \boldsymbol{v} = 0$, i.e., velocity is a *solenoidal* field. Let us try to express it in the form

$$\boldsymbol{v} = \nabla \times (\nabla \times \boldsymbol{e}_r \Phi) + \nabla \times \boldsymbol{e}_r \Psi \,, \tag{3.21}$$

where $\boldsymbol{e}_r$ is the unit vertical vector pointing against the direction of $\boldsymbol{g}_\circ$. We will suppose that in the cartesian geometry $\boldsymbol{e}_r$ is a constant vector and in the spherical geometry $\boldsymbol{e}_r$ is identical to the unit radial vector. It is clear that the equation of continuity (3.8) is fulfilled. The two "scalar potentials" Φ and Ψ define two components of the solenoidal field: the *poloidal* field $\boldsymbol{v}_P$ (generated by Φ) and the *toroidal* field $\boldsymbol{v}_T$ (generated by ψ).

It holds

$$\boldsymbol{v}_T \cdot \boldsymbol{e}_r = 0 \,, \tag{3.22}$$

i.e., the toroidal field is horizontal, and

$$(\nabla \times \boldsymbol{v}_P) \cdot \boldsymbol{e}_r = 0 \,. \tag{3.23}$$

Note that a general field can be decomposed into the toroidal field (satisfying the equation of continuity (3.8) together with the condition (3.22)) and the *spheroidal* field satisfying only (3.23).

3.1.5 Dimensionless variables

To simplify slightly the problem, we will now consider that reference density ρ_0, specific heat c_p, thermal conductivity k, gravity acceleration $\boldsymbol{g}_0$ and heat sources to be constant. This approximation is suitable for mantle convection modelling as the most changeable parameters in the mantle are probably viscosity and thermal expansion coefficient.

Let us introduce new dimensionless variables (denoted by the primes) by means of the relations

$$\boldsymbol{r} = d\boldsymbol{r}', \quad t = \frac{d^2}{\kappa}t', \quad \boldsymbol{v} = \frac{\kappa}{d}\boldsymbol{v}', \quad \Pi = \frac{\eta_s \kappa}{d^2}\Pi', \quad T = T_s + (T_b - T_s)T' \,, \tag{3.24}$$

where $\boldsymbol{r}$ is the position vector, d is the characteristic dimension of the system—e.g., the thickness of the mantle in mantle convection problems or the vertical dimension of the fluid layer in the problems in cartesian geometry—and η_s is a surface value of viscosity. The system (3.5), (3.6) and (3.8) in dimensionless variables thus reads

$$\nabla' \cdot \boldsymbol{v}' = 0 \,, \tag{3.25}$$

$$-\nabla'\Pi' + \nabla' \cdot \left(\frac{\eta}{\eta_s} (\nabla'\boldsymbol{v}' + (\nabla'\boldsymbol{v}')^T) \right) + \frac{\alpha_s (T_b - T_s) g_0 d^3}{\nu_s \kappa} \frac{\alpha}{\alpha_s} (T' - T_0') \boldsymbol{e}_r = \frac{\kappa}{\nu_s} \left(\frac{\partial \boldsymbol{v}'}{\partial t'} + \boldsymbol{v}' \cdot \nabla' \boldsymbol{v}' \right) \,, \tag{3.26}$$

where $\nu = \eta/\rho_0$ is the kinematic viscosity, and

$$\frac{\partial T'}{\partial t'} = \nabla'^2 T' - \boldsymbol{v}' \cdot \nabla' T' + \frac{Q d^2}{k(T_b - T_s)}$$

$$- \frac{\alpha_s g_0 d}{c_p} \left[\frac{\alpha}{\alpha_s} \left(T' + \frac{T_s}{T_b - T_s} \right) v'_r \right] + \frac{\eta_s \kappa}{\rho_0 c_p (T_b - T_s) d^2} \frac{\eta}{\eta_s} (\nabla' \boldsymbol{v}' + (\nabla' \boldsymbol{v}')^T) : \nabla' \boldsymbol{v}' . \quad (3.27)$$

We will be omitting the primes unless misunderstanding may arise.

The system (3.25)–(3.27) can be rewritten by means of the *dimensionless numbers* as

$$\nabla \cdot \boldsymbol{v} = 0 , \quad (3.28)$$

$$- \nabla \Pi + \nabla \cdot \left(\frac{\eta}{\eta_s} (\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T) \right) + Ra_s \frac{\alpha}{\alpha_s} (T - T_0) \boldsymbol{e}_r = Pr_s{}^{-1} \left(\frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v} \cdot \nabla \boldsymbol{v} \right) , \quad (3.29)$$

$$\frac{\partial T}{\partial t} = \nabla^2 T - \boldsymbol{v} \cdot \nabla T + \frac{Raq_s}{Ra_s} - D_s \frac{\alpha}{\alpha_s} \left(T + \frac{T_s}{T_b - T_s} \right) v_r + \frac{D_s}{Ra_s} \frac{\eta}{\eta_s} (\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T) : \nabla \boldsymbol{v} , \quad (3.30)$$

where we introduced

the (surface) Prandtl number	$Pr_s = \frac{\nu_s}{\kappa}$
the (surface) Rayleigh number	$Ra_s = \frac{\alpha_s (T_b - T_s) g_0 d^3}{\nu_s \kappa}$
the (surface) Rayleigh number for heat sources	$Raq_s = \frac{\alpha_s g_0 Q d^5}{\nu_s \kappa k}$
the (surface) dissipation number	$D_s = \frac{\alpha_s g_0 d}{c_p}$

.

In applications to mantle convection, the inertial force forming the r.h.s. of (3.29) is negligible. In other words, we may solve the system (3.28)–(3.30) for infinite Prandtl number; if we rewrite it for Θ instead of T, we get

$$\nabla \cdot \boldsymbol{v} = 0 , \quad (3.31)$$

$$- \nabla \Pi + \nabla \cdot \left(\frac{\eta}{\eta_s} (\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T) \right) + Ra_s \frac{\alpha}{\alpha_s} \Theta \boldsymbol{e}_r = 0 , \quad (3.32)$$

$$\frac{\partial \Theta}{\partial t} = \nabla^2 \Theta - \boldsymbol{v} \cdot \nabla T_0 - \boldsymbol{v} \cdot \nabla \Theta -$$

$$- D_s \frac{\alpha}{\alpha_s} \left(T_0 + \Theta + \frac{T_s}{T_b - T_s} \right) v_r + \frac{D_s}{Ra_s} \frac{\eta}{\eta_s} (\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T) : \nabla \boldsymbol{v} , \quad (3.33)$$

where T_0 is the conduction solution of the heat equation. The equations (3.31), (3.32) represent now an equilibrium system. In other words, time-dependence is not explicit and this system defines the mappings $\Theta \mapsto \boldsymbol{v}$ and $\Theta \mapsto \Pi$. This means that we may consider Θ as the only independent variable of the nonlinear equation

$$\frac{\partial \Theta}{\partial t} = \nabla^2 \Theta - \boldsymbol{v}(\Theta) \cdot \nabla T_0 - D_s \frac{\alpha}{\alpha_s} \left(T_0 + \frac{T_s}{T_b - T_s} \right) v_r(\Theta) - \boldsymbol{v}(\Theta) \cdot \nabla \Theta -$$

$$- D_s \frac{\alpha}{\alpha_s} \Theta v_r(\Theta) + \frac{D_s}{Ra_s} \frac{\eta}{\eta_s} (\nabla \boldsymbol{v}(\Theta) + (\nabla \boldsymbol{v}(\Theta))^T) : \nabla \boldsymbol{v}(\Theta) . \quad (3.34)$$

The classical Boussinesq approximation in dimensionless variables takes the form

$$\nabla \cdot \boldsymbol{v} = 0\,, \tag{3.35}$$

$$-\nabla\Pi + \nabla^2 \boldsymbol{v} + Ra\Theta\boldsymbol{e}_r = 0\,, \tag{3.36}$$

$$\frac{\partial\Theta}{\partial t} = \nabla^2\Theta - \boldsymbol{v}(\Theta)\cdot\nabla\Theta - \boldsymbol{v}(\Theta)\cdot\nabla T_0\,. \tag{3.37}$$

3.1.6 Fourier modes

In this section we will show how to use the Fourier technique to describe the full behaviour of the dynamical system (3.35)–(3.37). We will analyse the problem for free-slip impermeable boundary conditions (3.13), (3.14) and for the Dirichlet boundary conditions for temperature; $T = 0$ on the top and $T = 1$ on the bottom. This means that $\Theta = 0$ on these boundaries of the system. Let us study the two most usual geometries: cartesian and spherical.

Cartesian geometry

Here we will study a layer of a unit thickness perpendicular to gravity acceleration $\boldsymbol{g}_0$. This means that the plane $z = 0$ is the bottom and $z = 1$ is the top of the layer. We will employ the 2-D Fourier transform over x and y as in the previous chapter (see eqn. (**??**)). To satisfy the boundary conditions at the top and the bottom of the layer, we will decompose the unknown quantities as follows,

$$\hat{\Theta}(\boldsymbol{\lambda}, z; t) = \sum_{k=-\infty}^{\infty} i\hat{\Theta}_k(\boldsymbol{\lambda}; t)e^{ik\pi z}\,, \quad \hat{\Theta}_k = -\hat{\Theta}_{-k}\,, \tag{3.38}$$

$$\hat{v}_x(\boldsymbol{\lambda}, z; t) = \sum_{k=-\infty}^{\infty} i\hat{X}_k(\boldsymbol{\lambda}; t)e^{ik\pi z}\,, \quad \hat{X}_k = \hat{X}_{-k}\,, \tag{3.39}$$

$$\hat{v}_y(\boldsymbol{\lambda}, z; t) = \sum_{k=-\infty}^{\infty} i\hat{Y}_k(\boldsymbol{\lambda}; t)e^{ik\pi z}\,, \quad \hat{Y}_k = \hat{Y}_{-k}\,, \tag{3.40}$$

$$\hat{v}_z(\boldsymbol{\lambda}, z; t) = \sum_{k=-\infty}^{\infty} i\hat{Z}_k(\boldsymbol{\lambda}; t)e^{ik\pi z}\,, \quad \hat{Z}_k = -\hat{Z}_{-k}\,, \tag{3.41}$$

$$\hat{\Pi}(\boldsymbol{\lambda}, z; t) = \sum_{k=-\infty}^{\infty} \hat{\Pi}_k(\boldsymbol{\lambda}; t)e^{ik\pi z}\,, \tag{3.42}$$

where i is the imaginary unit, $\boldsymbol{\lambda}$ is the wavenumber vector corresponding to $\boldsymbol{r} = (x, y)$ and $\hat{\Theta}_k$, $\hat{X}_k$, $\hat{Y}_k$, $\hat{Z}_k$, $\hat{\Pi}_k$ are real-valued functions.

Eqn. (3.35) now reads

$$\boldsymbol{\lambda}\cdot\hat{\boldsymbol{u}}_k + k\pi\hat{Z}_k = 0\,, \tag{3.43}$$

where $\hat{\boldsymbol{u}}_k \equiv (\hat{X}_k, \hat{Y}_k)$. Similarly, eqn. (3.36) yields

$$\hat{\Pi}_k \boldsymbol{\lambda} + (\lambda^2 + k^2\pi^2)\hat{\boldsymbol{u}}_k = 0 \tag{3.44}$$

and

$$k\pi\hat{\Pi}_k + (\lambda^2 + k^2\pi^2)\hat{Z}_k = Ra\,\hat{\Theta}_k\,. \tag{3.45}$$

We can express $\hat{\boldsymbol{u}}_k$ from (3.44) and put it into (3.43). Then we easily obtain the solution

$$\hat{\boldsymbol{u}}_k = -\frac{k\pi\boldsymbol{\lambda}}{(\lambda^2 + k^2\pi^2)^2} Ra\,\hat{\Theta}_k\,, \tag{3.46}$$

$$\hat{Z}_k = \frac{\lambda^2}{(\lambda^2 + k^2\pi^2)^2} Ra\,\hat{\Theta}_k\,, \tag{3.47}$$

$$\hat{\Pi}_k = \frac{k\pi}{\lambda^2 + k^2\pi^2} Ra\,\hat{\Theta}_k\,. \tag{3.48}$$

Let us decompose $\hat{T}_0$ into the series,

$$\hat{T}_0 = \delta(\lambda_x)\delta(\lambda_y)\left((1-z) + \sum_{k=-\infty}^{\infty} i\hat{T}_{0,k}e^{ik\pi z}\right)\,, \quad \hat{T}_{0,k} = -\hat{T}_{0,-k}\,, \tag{3.49}$$

where δ represents the Dirac δ-function and $\hat{T}_{0,k}$ are the real numbers. The decomposition on the right-hand side has the following physical meaning: $(1-z)$ is the solution of the heat conduction equation with zero internal heating and non-zero boundary conditions, whereas the sum represents the solution of this equation with a homogeneous internal heating but with zero boundary conditions.

The *classical Boussinesq approximation* now reads

$$\frac{\partial\hat{\Theta}_n}{\partial t} = -(\lambda^2 + n^2\pi^2)\hat{\Theta}_n + \hat{Z}_n$$
$$+ \sum_k \left(\hat{X}_k * \lambda_x\hat{\Theta}_{n-k} + \hat{Y}_k * \lambda_y\hat{\Theta}_{n-k} + (n-k)\pi\hat{Z}_k * \hat{\Theta}_{n-k} + (n-k)\pi\hat{T}_{0,n-k}\hat{Z}_k\right)\,, \tag{3.50}$$

where the operator $*$ represents the 2-D convolution over the $\boldsymbol{\lambda}$-domain. If, moreover, there is *no internal heating*, we get

$$\frac{\partial\hat{\Theta}_n}{\partial t} = -(\lambda^2 + n^2\pi^2)\hat{\Theta}_n + \hat{Z}_n + \sum_k \left(\hat{X}_k * \lambda_x\hat{\Theta}_{n-k} + \hat{Y}_k * \lambda_y\hat{\Theta}_{n-k} + (n-k)\pi\hat{Z}_k * \hat{\Theta}_{n-k}\right)\,. \tag{3.51}$$

In more details,

$$\frac{\partial\hat{\Theta}_n}{\partial t} = -(\lambda^2 + n^2\pi^2)\,\hat{\Theta}_n + \frac{\lambda^2\,Ra}{(\lambda^2 + n^2\pi^2)^2}\,\hat{\Theta}_n +$$
$$\sum_k \pi\,Ra\left(\frac{-k\lambda_x\hat{\Theta}_k}{(\lambda^2 + k^2\pi^2)^2} * (\lambda_x\hat{\Theta}_{n-k}) + \frac{-k\lambda_y\hat{\Theta}_k}{(\lambda^2 + k^2\pi^2)^2} * (\lambda_y\hat{\Theta}_{n-k}) + \frac{(n-k)\lambda^2\hat{\Theta}_k}{(\lambda^2 + k^2\pi^2)^2} * \hat{\Theta}_{n-k}\right)\,. \tag{3.52}$$

3.1.7 Onset of convection

This section deals with the study of situations when the state of the dynamical system (3.34) corresponding to the transfer of heat by pure conduction becomes unstable and fluctuations in the system result in convection. Since the purely conductive state is represented simply by $\Theta = 0$, its stability is given by the behaviour of the linear part of (3.34). We can use the linear part of the classical Boussinesq approximation (3.50) and add the term $-D_s(T_0 + T_s/(T_b - T_s))v_z(\Theta)$ from (3.34). For simplicity, in the next considerations we will assume that both viscosity and thermal expansion coefficient are constant (that is why we will write Ra and D instead of Ra_s and D_s, respectively).

Now we can start with rewriting the linear part of (3.34) into the modal form if $D \neq 0$. The Fourier transform of the l.h.s. of (3.34) $\partial\hat{\Theta}/\partial t = \sum_k i(\partial\hat{\Theta}_k/\partial t)\exp(ik\pi z)$ is the sine series owing to the symmetry $\hat{\Theta}_k = -\hat{\Theta}_{-k}$. This is the reason why we also need to express the term $T_0 v_z$ by means of the sine series.

It is easy to decompose $(1-z)$ into the cosine series and to get from (3.49)

$$\hat{T}_0 = \left(\frac{1}{2} + \sum_{k=-\infty,k\neq 0}^{\infty} \frac{(-1)^k - 1}{k^2\pi^2} e^{ik\pi z}\right)\delta(\lambda_x)\delta(\lambda_y) + \sum_{k=-\infty}^{\infty} i\hat{T}_{0,k}e^{ik\pi z}\,, \quad \hat{T}_{0,k} = -\hat{T}_{0,-k}\,, \tag{3.53}$$

The vertical component of velocity v_z is decomposed into the sine series (3.41). The part of T_0 expressing the influence of internal heating is expressed by means of the sine series and thus we will have to deal with the product of this two sine series as follows,

$$\hat{v}_z * \sum_{k=-\infty}^{\infty} i\hat{T}_{0,k}e^{ik\pi z} = \sum_{k=-\infty}^{\infty}\sum_{j=-\infty}^{\infty} -\hat{Z}_j * \hat{T}_{0,k-j}e^{ik\pi z} = \sum_{k\geq 0}^{\infty}\sum_{j=-\infty}^{\infty} -\hat{Z}_j * \hat{T}_{0,k-j} 2\cos k\pi z\,. \tag{3.54}$$

Since

$$\int_0^1 \cos k\pi z\, \sin n\pi z\, dz = \frac{1}{n\pi}\left[-\cos k\pi z\, \cos n\pi z\right]_0^1 - \frac{k}{n}\int_0^1 \sin k\pi z\, \cos n\pi z\, dz =$$

$$= \frac{(-1)^{k+n+1} + 1}{n\pi} + \frac{k^2}{n^2}\int_0^1 \cos k\pi z\, \sin n\pi z\, dz\,,$$

we obtain

$$\int_0^1 \cos k\pi z\, \sin n\pi z\, dz = \begin{cases} \frac{n((-1)^{k+n}-1)}{\pi(k^2-n^2)} & n \neq k \\ 0 & n = k \end{cases}\,.$$

Taking into account the norms $\int_0^1 \sin^2 n\pi z\, dz = \frac{1}{2}$, we can finally write

$$-2\cos k\pi z = \sum_{n=1,n\neq k} -[(-1)^{k+n} - 1]\frac{4n}{(k^2-n^2)\pi}\sin n\pi z =$$

$$= \sum_{n=-\infty,|n|\neq k}^{\infty} i[(-1)^{k+|n|}-1]\frac{2n}{(k^2-n^2)\pi}e^{in\pi z}\,,$$

which implies that

$$\hat{v}_z * \sum_{k=-\infty}^{\infty} i\hat{T}_{0,k}e^{ik\pi z} = \sum_{n=-\infty}^{\infty} i\left(\sum_{k\geq 0,k\neq|n|}^{\infty}[(-1)^{k+|n|}-1]\frac{2n}{(k^2-n^2)\pi}\sum_{j=-\infty}^{\infty}\hat{Z}_j * \hat{T}_{0,k-j}\right)e^{in\pi z}\,. \tag{3.55}$$

As already written above, the conduction solution is given simply by zero-point in the space of state vectors $\vec{\Theta}$, i.e.

$$\vec{\Theta} = \vec{0}\,. \tag{3.56}$$

If a fluctuation $\vec{\Theta}\neq 0,\ ||\vec{\Theta}|| \ll 1$ appears, the start of its evolution may be approximated by linearized version of (3.34),

$$\frac{\partial\,\vec{\Theta}(\boldsymbol{\lambda})}{\partial t} = \mathcal{A}(\lambda)\vec{\Theta}(\boldsymbol{\lambda})\,. \tag{3.57}$$

It follows from (3.50) and from the fact that the constant part of $(T_0 + T_s/(T_b - T_s))$ in (3.34) is $\frac{1}{2}(T_b+T_s)/(T_b-T_s)$ according to (3.53) that the diagonal part of $\mathcal{A}$ is

$$\mathcal{A}_{nn}(\lambda) = -(\lambda^2+n^2\pi^2) + \left(1-\frac{D}{2}\frac{T_b+T_s}{T_b-T_s}\right)\frac{\lambda^2\,Ra}{(\lambda^2+n^2\pi^2)^2}\,. \tag{3.58}$$

Simultaneously, (3.50), (3.53) and (3.55) yield

$$\mathcal{A}_{nk}(\boldsymbol{\lambda}) = -D\frac{(-1)^{n-k}-1}{(n-k)^2\pi^2}\frac{\lambda^2\,Ra}{(\lambda^2+k^2\pi^2)^2}$$

$$+\pi\,Ra\left(\frac{-k\lambda_x}{(\lambda^2+k^2\pi^2)^2} * (\lambda_x\hat{T}_{0,n-k}) + \frac{-k\lambda_y}{(\lambda^2+k^2\pi^2)^2} * (\lambda_y\hat{T}_{0,n-k}) + \frac{(n-k)\lambda^2}{(\lambda^2+k^2\pi^2)^2} * \hat{T}_{0,n-k}\right)$$

$$-\,D\sum_{j\geq 0,j\neq|n|}^{\infty}[(-1)^{j+|n|}-1]\frac{2n}{(j^2-n^2)\pi}\left(\frac{\lambda^2\,Ra}{(\lambda^2+k^2\pi^2)^2}\right) * \hat{T}_{0,j-k}\,,\quad n\neq k\,. \tag{3.59}$$

The solution of (3.58)–(3.59) is

$$\vec{\Theta}(\boldsymbol{\lambda}) = \vec{C}\,\exp(\mathcal{A}(\boldsymbol{\lambda})t)\,, \tag{3.60}$$

where $\vec{C}$ is the vector of integration constants. If real parts of all eigenvalues of $\mathcal{A}(\boldsymbol{\lambda})$ are negative for any wavenumber vector $\boldsymbol{\lambda}$, (3.60) represents the solution of exponentially damped system. From the physical point of view, this means that all fluctuations disappear after some time and the conductive solution is thus stable. However, if there exist such $\boldsymbol{\lambda}$ that at least one eigenvalue has positive real part, then fluctuations of the corresponding wavelength can be amplified.

To study the problem in more details, let us confine to the classical Boussinesq approximation ($D = 0$) with no internal heating ($\hat{T}_{0,k} = 0 \ \forall k$). In this case the matrix $\mathcal{A}$ is diagonal, its eigenvalues are

$$\beta_n(\lambda) = -(\lambda^2 + n^2\pi^2) + \frac{\lambda^2 \, Ra}{(\lambda^2 + n^2\pi^2)^2} \tag{3.61}$$

and $\beta_1 > \beta_2 > \beta_3 \ldots$. Therefore, in this stability analysis it is sufficient to deal with β_1 only. It is clear that $\beta_1 < 0 \ \forall\lambda \Leftrightarrow Ra < (\lambda^2 + \pi^2)^3/\lambda^2 \ \forall\lambda$. Let us find the minimum of the function $f(\lambda) = (\lambda^2 + \pi^2)^3/\lambda^2$. As $\partial f/\partial\lambda = \lambda^{-4}(6\lambda^3(\lambda^2 + \pi^2)^2 - 2\lambda(\lambda^2 + \pi^2)^3)$, f attains its minimum in $\lambda_m = \pi/\sqrt{2}$; $f(\lambda_m) = \frac{27}{4}\pi^4$. To conclude: if

$$Ra < Ra_c = \frac{27}{4}\pi^4 , \tag{3.62}$$

the transfer of heat due to conduction represents the stable state and no convection arises. However, if the Rayleigh number is greater than the *critical Rayleigh number* Ra_c, convection is generated by fluctuations in the system.

3.2 2-D problems

To study the basic physics of various problems, it is often sufficient to use only 2-D approximations when we suppose that the flow does not depend on one of the dimensions. This approach saves a lot of computer requirements and enables thus to solve thermal convection problems even on PCs. Moreover, because of the equation of continuity, the convection can be fully described by a scalar function in such a case. We will again concentrate on the two geometries which are usually used in geophysics: cartesian and spherical.

3.2.1 Cartesian geometry

Let us suppose that velocity does not depend on the y-coordinate and that $v_y = 0$. In this case, we can obtain the solenoidal field satisfying the equation of continuity ($\nabla \cdot \boldsymbol{v} = 0$) by expressing velocity in the form

$$\boldsymbol{v} \equiv (v_x, v_z) = \left(\frac{\partial\psi}{\partial z}, -\frac{\partial\psi}{\partial x}\right) , \tag{3.63}$$

where $\psi = \psi(x, z)$ is the *stream function.* As

$$\boldsymbol{v} \cdot \nabla\psi = 0 , \tag{3.64}$$

it is clear that the isolines of ψ are the streamlines of velocity.

The momentum equation(3.32) can be now rewritten to

$$-\frac{\partial \Pi}{\partial x} + \frac{\partial}{\partial x}\left[2\frac{\eta}{\eta_s}\frac{\partial v_x}{\partial x}\right] + \frac{\partial}{\partial z}\left[\frac{\eta}{\eta_s}\left(\frac{\partial v_x}{\partial z} + \frac{\partial v_z}{\partial x}\right)\right] = 0\,, \tag{3.65}$$

$$-\frac{\partial \Pi}{\partial z} + \frac{\partial}{\partial z}\left[2\frac{\eta}{\eta_s}\frac{\partial v_z}{\partial z}\right] + \frac{\partial}{\partial x}\left[\frac{\eta}{\eta_s}\left(\frac{\partial v_x}{\partial z} + \frac{\partial v_z}{\partial x}\right)\right] = -Ra_s\frac{\alpha}{\alpha_s}\Theta\,, \tag{3.66}$$

or, in the stream function formulation,

$$-\frac{\partial \Pi}{\partial x} + \frac{\partial}{\partial x}\left[2\frac{\eta}{\eta_s}\frac{\partial^2 \psi}{\partial x \partial z}\right] + \frac{\partial}{\partial z}\left[\frac{\eta}{\eta_s}\left(\frac{\partial^2 \psi}{\partial z^2} - \frac{\partial^2 \psi}{\partial x^2}\right)\right] = 0\,, \tag{3.67}$$

$$-\frac{\partial \Pi}{\partial z} - \frac{\partial}{\partial z}\left[2\frac{\eta}{\eta_s}\frac{\partial^2 \psi}{\partial x \partial z}\right] + \frac{\partial}{\partial x}\left[\frac{\eta}{\eta_s}\left(\frac{\partial^2 \psi}{\partial z^2} - \frac{\partial^2 \psi}{\partial x^2}\right)\right] = -Ra_s\frac{\alpha}{\alpha_s}\Theta\,, \tag{3.68}$$

After applying the operator $\partial/\partial z$ to (3.67), the operator $\partial/\partial x$ to (3.68), and subtracting both equations we obtain the final form of the momentum equation

$$\left(\frac{\partial^2}{\partial z^2} - \frac{\partial^2}{\partial x^2}\right)\left[\frac{\eta}{\eta_s}\left(\frac{\partial^2 \psi}{\partial z^2} - \frac{\partial^2 \psi}{\partial x^2}\right)\right] + 4\frac{\partial^2}{\partial x \partial z}\left[\frac{\eta}{\eta_s}\frac{\partial^2 \psi}{\partial x \partial z}\right] = Ra_s\frac{\partial}{\partial x}\left[\frac{\alpha}{\alpha_s}\Theta\right]. \tag{3.69}$$

The heat equation (3.33) reads

$$\frac{\partial \Theta}{\partial t} = \nabla^2\Theta - \frac{\partial \psi}{\partial z}\frac{\partial}{\partial x}(T_0 + \Theta) + \frac{\partial \psi}{\partial x}\frac{\partial}{\partial z}(T_0 + \Theta)$$

$$+ D_s\frac{\alpha}{\alpha_s}\left(T_0 + \Theta + \frac{T_s}{T_b - T_s}\right)\frac{\partial \psi}{\partial x} + \frac{D_s}{Ra_s}\frac{\eta}{\eta_s}\left[\left(\frac{\partial^2 \psi}{\partial z^2} - \frac{\partial^2 \psi}{\partial x^2}\right)^2 + 4\left(\frac{\partial^2 \psi}{\partial x \partial z}\right)^2\right]. \tag{3.70}$$

For the classical Boussinesq approximation without internal heating the system (3.69), (3.70) simplifies to

$$\nabla^4\psi = Ra\frac{\partial \Theta}{\partial x}\,, \tag{3.71}$$

$$\frac{\partial \Theta}{\partial t} = \nabla^2\Theta - \frac{\partial \psi}{\partial z}\frac{\partial \Theta}{\partial x} + \frac{\partial \psi}{\partial x}\frac{\partial \Theta}{\partial z} - \frac{\partial \psi}{\partial x}\,. \tag{3.72}$$

If we consider impermeable, free-slip boundary conditions for $z = 0$ and $z = 1$, we obtain the boundary conditions in the form:

$$\psi = \frac{\partial^2 \psi}{\partial z^2} = 0 \quad \text{for} \quad z = 0, 1\,. \tag{3.73}$$

We can again convert the problem into the spectral domain by applying the Fourier transform and sine decomposition as follows,

$$\hat{\psi}(\lambda; z, t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi(x; z, t)e^{-i\lambda x}\,dx\,, \tag{3.74}$$

$$\hat{\psi}(\lambda; z, t) = \sum_{n=-\infty}^{\infty} \hat{\psi}_n(\lambda; t) e^{in\pi z}\,, \quad \hat{\psi}_n = -\hat{\psi}_{-n}\,, \tag{3.75}$$

$$\hat{\Theta}(\lambda; z, t) = \sum_{n=-\infty}^{\infty} i\hat{\Theta}_n(\lambda; t) e^{in\pi z}\,, \quad \hat{\Theta}_n = -\hat{\Theta}_{-n}\,. \tag{3.76}$$

The solution of the biharmonic equation (3.71) in the spectral domain is

$$\hat{\psi}_n = \frac{-\lambda\, Ra}{(\lambda^2 + n^2\pi^2)^2}\, \hat{\Theta}_n\,. \tag{3.77}$$

In the case of no internal heating $T_0 = 1 - z$, and thus the heat equation (3.72) attains the form

$$\frac{\partial \hat{\Theta}_n}{\partial t} = -(\lambda^2 + n^2\pi^2)\,\hat{\Theta}_n + \frac{\lambda^2\, Ra}{(\lambda^2 + n^2\pi^2)^2}\,\hat{\Theta}_n$$
$$+ \sum_k \pi\, Ra \left(\frac{-k\lambda\hat{\Theta}_k}{(\lambda^2 + k^2\pi^2)^2} * (\lambda\hat{\Theta}_{n-k}) + \frac{(n-k)\lambda^2\hat{\Theta}_k}{(\lambda^2 + k^2\pi^2)^2} * \hat{\Theta}_{n-k} \right)\,, \tag{3.78}$$

where the operator $*$ means the 1-D convolution over x now.

3.2.2 Spherical geometry

In this section we will deal with the axisymmetric flow

$$\boldsymbol{v} \equiv (v_r, v_\vartheta, v_\varphi) = (v_r(r,\vartheta), v_\vartheta(r,\vartheta), 0) \tag{3.79}$$

confined between two spherical surfaces with the radii r_1 and r_2. Here r, ϑ and φ are the spherical coordinates. For simplicity, we will consider only depth-dependence of viscosity and thermal expansivity, i.e. the momentum equation attains the form

$$\nabla\cdot\boldsymbol{\sigma} - \nabla\Pi = -Ra_s\alpha'(r)\Theta\boldsymbol{e}_r\,, \tag{3.80}$$

$$\boldsymbol{\sigma} = \eta'(r)(\nabla\boldsymbol{v} + (\nabla\boldsymbol{v})^T)\,, \tag{3.81}$$

where

$$\alpha' \equiv \frac{\alpha}{\alpha_s}\,, \quad \eta' \equiv \frac{\eta}{\eta_s}\,.$$

Due to the equation of continuity (3.31), $\nabla\cdot(\nabla\boldsymbol{v})^T = 0$ and thus

$$\nabla\cdot\boldsymbol{\sigma} = \eta'\nabla\cdot\nabla\boldsymbol{v} + \nabla\eta'\cdot(\nabla\boldsymbol{v} + (\nabla\boldsymbol{v})^T) = -\eta'\nabla\times\nabla\times\boldsymbol{v} + \nabla\eta'\cdot(\nabla\boldsymbol{v} + (\nabla\boldsymbol{v})^T)\,, \tag{3.82}$$

i.e. the momentum equation (3.80) may be written as

$$-\eta'\nabla\times\nabla\times\boldsymbol{v} + \nabla\eta'\cdot(\nabla\boldsymbol{v} + (\nabla\boldsymbol{v})^T) - \nabla\Pi = -Ra_s\alpha'(r)\Theta\boldsymbol{e}_r\,. \tag{3.83}$$

Rotation of a vector field $\boldsymbol{u}$ expressed in the spherical coordinates is

$$\nabla \times \boldsymbol{u} = \frac{1}{r \sin\vartheta} \left(\frac{\partial (u_\varphi \sin\vartheta)}{\partial \vartheta} - \frac{\partial u_\vartheta}{\partial \varphi} \,,\; \frac{\partial u_r}{\partial \varphi} - \sin\vartheta \frac{\partial (r u_\varphi)}{\partial r} \,,\; \sin\vartheta \frac{\partial (r u_\vartheta)}{\partial r} - \sin\vartheta \frac{\partial u_r}{\partial \vartheta} \right) . \tag{3.84}$$

Therefore, after applying the operator $r \sin\vartheta\, \nabla\times$ to (3.83) we get

$$-r \sin\vartheta\, \nabla\times[\eta'(r) \nabla\times\nabla\times\boldsymbol{v}] + r \sin\vartheta\, \nabla\times[\nabla\eta'(r)\cdot(\nabla\boldsymbol{v}+(\nabla\boldsymbol{v})^T)] = (0 \,,\, 0 \,,\, Ra_s \alpha'(r) \sin\vartheta \, \frac{\partial \Theta}{\partial \vartheta}) . \tag{3.85}$$

Let ω be the φ-th component of *vorticity* $\nabla \times \boldsymbol{v}$ multiplied by $r \sin\vartheta$, i.e.,

$$\nabla \times \boldsymbol{v} = (0 \,,\, 0 \,,\, \frac{\omega}{r \sin\vartheta}) , \tag{3.86}$$

and let $\mathcal{D}$ be the Laplacian-like operator

$$\mathcal{D} \equiv \frac{\partial^2}{\partial r^2} + \sin\vartheta \frac{\partial}{\partial \vartheta} \frac{1}{r^2 \sin\vartheta} \frac{\partial}{\partial \vartheta} = \frac{\partial^2}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2}{\partial \vartheta^2} - \frac{\cos\vartheta}{r^2 \sin\vartheta} \frac{\partial}{\partial \vartheta} . \tag{3.87}$$

Then

$$-r \sin\vartheta\, \nabla \times [\eta'(r) \nabla \times \nabla \times \boldsymbol{v}] = -r \sin\vartheta\, \nabla \times \left(\frac{\eta'}{r^2 \sin\vartheta} \frac{\partial \omega}{\partial \vartheta} \,,\; -\frac{\eta'}{r \sin\vartheta} \frac{\partial \omega}{\partial r} \,,\; 0 \right) =$$

$$= \left(0 \,,\, 0 \,,\, \frac{\partial}{\partial r}(\eta' \frac{\partial \omega}{\partial r}) + \frac{\sin\vartheta}{r^2} \frac{\partial}{\partial \vartheta}(\frac{\eta'}{\sin\vartheta} \frac{\partial \omega}{\partial \vartheta}) \right) = \left(0 \,,\, 0 \,,\, \mathcal{D}(\eta'\omega) - \frac{\partial \eta'}{\partial r} \frac{\partial \omega}{\partial r} - \frac{\partial^2 \eta'}{\partial r^2} \omega \right) . \tag{3.88}$$

Let us introduce again the *stream function* ψ so that velocity should satisfy the equation of continuity:

$$\boldsymbol{v} = (v_r(r,\vartheta) \,,\, v_\vartheta(r,\vartheta) \,,\, 0) = (\frac{1}{r^2 \sin\vartheta} \frac{\partial \psi}{\partial \vartheta} \,,\; -\frac{1}{r \sin\vartheta} \frac{\partial \psi}{\partial r} \,,\; 0) \tag{3.89}$$

The relations (3.84), (3.86), (3.87) and (3.89) yield

$$-\,\omega = -\sin\vartheta (\frac{\partial}{\partial r}(r v_\vartheta) - \frac{\partial v_r}{\partial \vartheta}) = \frac{\partial^2 \psi}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2 \psi}{\partial \vartheta^2} - \frac{\cos\vartheta}{r^2 \sin\vartheta} \frac{\partial \psi}{\partial \vartheta} = \mathcal{D}(\psi) , \tag{3.90}$$

We may thus rewrite (3.88) as follows,

$$-\, r \sin\vartheta\, \nabla \times [\eta'(r) \nabla \times \nabla \times \boldsymbol{v}] = \left(0 \,,\, 0 \,,\, \mathcal{D}(\eta'\omega) + \frac{\partial \eta'}{\partial r} \frac{\partial}{\partial r} \mathcal{D}(\psi) + \frac{\partial^2 \eta'}{\partial r^2} \mathcal{D}(\psi) \right) . \tag{3.91}$$

Since

$$\nabla \eta' = (\frac{\partial \eta'}{\partial r} \,,\, 0 \,,\, 0) , \tag{3.92}$$

$$(\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T)_{rr} = 2 \frac{\partial v_r}{\partial r} \,, \quad (\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T)_{r\vartheta} = \frac{1}{r} \frac{\partial v_r}{\partial \vartheta} + \frac{\partial v_\vartheta}{\partial r} - \frac{v_\vartheta}{r} , \tag{3.93}$$

we have

$$\nabla\eta' \cdot (\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T) = \left(2\frac{\partial \eta'}{\partial r}\frac{\partial v_r}{\partial r} \;,\; \frac{\partial \eta'}{\partial r}(\frac{1}{r}\frac{\partial v_r}{\partial \vartheta} + \frac{\partial v_\vartheta}{\partial r} - \frac{v_\vartheta}{r}) \;,\; 0 \right) . \tag{3.94}$$

Now we are able to express the second term on the l.h.s. of (3.85) in the following form:

$$r \sin\vartheta \, \nabla \times [\nabla\eta'(r) \cdot (\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T)]$$

$$= \left(0 \;,\; 0 \;,\; \sin\vartheta \left[(\frac{\partial^2 v_r}{\partial r \partial \vartheta} + r\frac{\partial^2 v_\vartheta}{\partial r^2})\frac{\partial \eta'}{\partial r} + \frac{\partial^2 \eta'}{\partial r^2}(\frac{\partial v_r}{\partial \vartheta} + r\frac{\partial v_\vartheta}{\partial r} - v_\vartheta) - 2\frac{\partial \eta'}{\partial r}\frac{\partial^2 v_r}{\partial r \partial \vartheta} \right] \right)$$

$$= \left(0 \;,\; 0 \;,\; \sin\vartheta \left[\left((\frac{\partial}{\partial r}\frac{1}{r^2}(\frac{\cos\vartheta}{\sin^2\vartheta}\frac{\partial \psi}{\partial \vartheta} - \frac{1}{\sin\vartheta}\frac{\partial^2 \psi}{\partial \vartheta^2}) + r\frac{\partial}{\partial r}\frac{1}{\sin\vartheta}(\frac{1}{r^2}\frac{\partial \psi}{\partial r} - \frac{1}{r}\frac{\partial^2 \psi}{\partial r^2}) \right) \frac{\partial \eta'}{\partial r} \right.\right.$$

$$\left.\left. + \left(\frac{1}{r^2}(-\frac{\cos\vartheta}{\sin^2\vartheta}\frac{\partial \psi}{\partial \vartheta} + \frac{1}{\sin\vartheta}\frac{\partial^2 \psi}{\partial \vartheta^2}) + \frac{r}{\sin\vartheta}(\frac{1}{r^2}\frac{\partial \psi}{\partial r} - \frac{1}{r}\frac{\partial^2 \psi}{\partial r^2} + \frac{1}{r^2}\frac{\partial \psi}{\partial r}) \right) \frac{\partial^2 \eta'}{\partial r^2} \right] \right)$$

$$= \left(0 \;,\; 0 \;,\; \left(-\frac{\partial}{\partial r}\mathcal{D}(\psi) + \frac{\partial}{\partial r}(\frac{2}{r}\frac{\partial \psi}{\partial r}) \right) \frac{\partial \eta'}{\partial r} + \left(\mathcal{D}(\psi) - 2\frac{\partial^2 \psi}{\partial r^2} + \frac{2}{r}\frac{\partial \psi}{\partial r} \right) \frac{\partial^2 \eta'}{\partial r^2} \right) . \tag{3.95}$$

Eqns. (3.85), (3.90), (3.91) and (3.95) yield the final momentum equation in the vorticity-stream function formulation as follows,

$$\mathcal{D}(\eta'\omega) = Ra_s \alpha' \sin\vartheta \frac{\partial \Theta}{\partial \vartheta} - 2\frac{\partial^2 \eta'}{\partial r^2} \sin\vartheta \frac{\partial}{\partial \vartheta} \left(\frac{1}{r^2 \sin\vartheta}\frac{\partial \psi}{\partial \vartheta} \right) - \frac{\partial}{\partial r} \left(\frac{2}{r}\frac{\partial \psi}{\partial r}\frac{\partial \eta'}{\partial r} \right) , \tag{3.96}$$

$$\mathcal{D}(\psi) = -\omega \, . \tag{3.97}$$

The system (3.96), (3.97) must be completed by boundary conditions. We will consider here impermeable, free-slip spherical boundaries, i.e. the flow on the boundaries is characterized by the relations

$$v_r = 0 \;, \quad \sigma_{r\vartheta} = 0 \, . \tag{3.98}$$

It follows from (3.89) that the conditions $v_r = 0$ can be easily satisfied by putting

$$\psi = 0 \tag{3.99}$$

on the boundaries. Analogically, it follows from (3.93) that there is a free-slip on the boundary if

$$\frac{1}{r}\frac{\partial v_r}{\partial \vartheta} + \frac{\partial v_\vartheta}{\partial r} - \frac{v_\vartheta}{r} = 0 \, ,$$

i.e.,

$$\frac{1}{r}\frac{\partial}{\partial \vartheta} \left(\frac{1}{r^2 \sin\vartheta}\frac{\partial \psi}{\partial \vartheta} \right) - \frac{\partial}{\partial r} \left(\frac{1}{r \sin\vartheta}\frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin\vartheta}\frac{\partial \psi}{\partial r} \, ,$$

which may be written as

$$\mathcal{D}(\psi) = \frac{2}{r}\frac{\partial \psi}{\partial r} \, . \tag{3.100}$$

If we take into account the relation (3.97), we get the boundary condition for vorticity in the form

$$\omega = -\frac{2}{r}\frac{\partial \psi}{\partial r} \, . \tag{3.101}$$

3.3 Nonlinear dynamics

In the previous section the thermal convection in a layer was studied by means of the decomposition of temperature into the discrete set of the Fourier modes. The discretization was the consequence of the finite dimension of the studied geometry in the vertical direction. However, each mode was a function of the continuously changing wavenumber vector $\boldsymbol{\lambda}$ because the system was not bounded in horizontal directions. To simplify the problem, we will confine here to the thermal convection in bounded domains in all directions to deal with purely discrete modes.

For example, if we study the 2-D convection in a cartesian box with the impermeable and free-slip thermally isolating ($\partial T/\partial x = 0$) sidewalls at $x = 0$ and $x = d$, we can also decompose the stream function and thermal modes defined respectively in (3.75) and (3.76) and to get

$$\hat{\psi}_n = \sum_{m=-\infty}^{\infty} \hat{\psi}_{mn}(t) e^{im\pi\frac{x}{d}} , \quad \hat{\psi}_{mn} = -\hat{\psi}_{-m,n} , \quad \hat{\psi}_{mn} = -\hat{\psi}_{m,-n} , \tag{3.102}$$

$$\hat{\Theta}_n = \sum_{m=-\infty}^{\infty} \hat{\Theta}_{mn}(t) e^{im\pi\frac{x}{d}} , \quad \hat{\Theta}_{mn} = \hat{\Theta}_{-m,n} , \quad \hat{\Theta}_{mn} = -\hat{\Theta}_{m,-n} . \tag{3.103}$$

The equations (3.77), (3.78) are then replaced by

$$\hat{\psi}_{mn} = \frac{-md^3\, Ra}{\pi^3(m^2+n^2d^2)^2}\, \hat{\Theta}_{mn} \tag{3.104}$$

and

$$\frac{d\hat{\Theta}_{mn}}{dt} = -\frac{\pi^2}{d^2}(m^2+n^2d^2)\, \hat{\Theta}_{mn} + \frac{m^2d^2\, Ra}{\pi^2(m^2+n^2d^2)^2}\, \hat{\Theta}_{mn}$$
$$+ \sum_{kl} \frac{d^2\, Ra}{\pi(l^2+k^2d^2)^2} \left(-kl(m-l) + l^2(n-k)\right) \hat{\Theta}_{lk} \hat{\Theta}_{m-l,n-k} . \tag{3.105}$$

If we take into account only finite number of modes, we obtain a system, which can formally be written as

$$\frac{dw_i}{dt} = F_i(\mathbf{w}, Ra) , \quad i = 1, 2, ..., N , \tag{3.106}$$

where w_i are the coordinates of the phase-space formed by the N selected modes and Ra represents the controlling parameter of the non-linear dynamical system. If we choose any point $\boldsymbol{w}_0 \in E_N$ representing a particular state of the studied dynamical system, we can obtain the evolution path starting from $\boldsymbol{w}_0$ by solving the system (3.106) with the initial condition $\boldsymbol{w} = \boldsymbol{w}_0$. In other words, the solution of (3.106) defines the operator

$$f^t : E_N \mapsto E_N , \quad f^s \circ f^t = f^{s+t} , \tag{3.107}$$

Since the system (3.106) is deterministic and enables, in principle, the study of the past by changing the sign of time, it must hold $f^{-t} = (f^t)^{-1}$ and thus f^0 is the identity operator.

Let us deal with the evolution of a volume dV in the phase-space corresponding to the system (3.105). As $\hat{\Theta}_{k,0} = 0$,

$$\sum_{mn} \frac{\partial}{\partial \hat{\Theta}_{mn}} \left(\frac{d\hat{\Theta}_{mn}}{dt} \right) = \sum_{mn} -\frac{\pi^2}{d^2}(m^2 + n^2 d^2) + \frac{m^2 d^2\, Ra}{\pi^2 (m^2 + n^2 d^2)^2} \, . \tag{3.108}$$

This means that if we take into account a sufficient number of modes (in principle, there is the infinite number of modes), then $dV/dt < 0$, i.e., the phase-space volume decreases during the time evolution. Nonlinear dynamical systems with this property are called *dissipative*. This, however, does not mean that the volume dV must contract in all directions. The modes satisfying the condition

$$-\frac{\pi^2}{d^2}(m^2 + n^2 d^2) + \frac{m^2 d^2\, Ra}{\pi^2 (m^2 + n^2 d^2)^2} > 0 \tag{3.109}$$

correspond to the phase-space directions of dV dilatations during its time evolution along the evolution path. The consequence of dissipation is that there may be a set of states (points in the phase-space) which is asymptotically reached for long positive times by all evolution paths. This property is specified in the next definition.

Definition:
The attracting set A with the fundamental neighbourhood U satisfies the following properties

1. $A \subset U$, U is open.
2. For any open $V \supset A$ there exists $t > 0$ such that $f^t(U) \subset V$.
3. $f^t(A) = A \ \forall t$.

The domain of influence of the attracting set A is $\bigcup_{t<0} f^t(U)$. If the domain of influence is the whole phase-space, we call A to be *the universal attracting set.* [1]

Let $w_i(t; \mathbf{w}_0)$ is the evolution path satisfying (3.106) with the initial condition $\mathbf{w} = \mathbf{w}_0$ at $t = 0$. Employing the Taylor expansion to (3.106), we may write

$$w_i(t; \mathbf{w}_0 + \delta \mathbf{w}_0) \doteq w_i(t; \mathbf{w}_0) + \sum_{j=1}^{N} \frac{\partial w_i}{\partial w_{0_j}}(t; \mathbf{w}_0) \delta w_{0j} \ , \tag{3.110}$$

[1] Let U_1 and U_2 be two fundamental neighbourhoods of the attracting set A. Then there exists $s > 0$ such that $f^s(U_1) \subset U_2$. Therefore, $f^t(U_2) \supset f^{t+s}(U_1)$ for any $t \in E_1$. It holds $\bigcup_{t<0} f^t(U_2) \supset \bigcup_{t<-s} f^t(U_2) \supset \bigcup_{t<-s} f^{t+s}(U_1) = \bigcup_{t<0} f^t(U_1)$. By changing U_1 with U_2 we can analogically prove $\bigcup_{t<0} f^t(U_1) \supset \bigcup_{t<0} f^t(U_2)$, which means that the domain of influence does not depend on the choice of the fundamental neighbourhood.

where

$$\Pi_{ij}(t;\mathbf{w}_0) \equiv \frac{\partial w_i}{\partial w_{0_j}}(t;\mathbf{w}_0) \tag{3.111}$$

is the propagator matrix of the selected evolution path. The expansion (3.110) can be thus rewritten into the form

$$\delta\mathbf{w}(t;\mathbf{w}_0;\delta\mathbf{w}_0) \doteq \boldsymbol{\Pi}(t;\mathbf{w}_0)\cdot\delta\mathbf{w}_0 \ . \tag{3.112}$$

The *Lyapunov exponents* λ_i may be then defined by the relation

$$\boxed{\lambda_i = \lim_{t\to\infty}\sup \tfrac{1}{t}\ln|\alpha_i(t)|} \ , \tag{3.113}$$

where $\alpha_i(t)$ are the characteristic values of the propagator matrix.

The Lyapunov exponents represent the rate of exponential growth or damping of infinitesimal displacements with time, i.e., the inverse of the highest positive Lyapunov exponent gives the characteristic time of predictability of a selected evolution path. To demonstrate such an exponential behaviour, suppose that F_i are smooth enough and expand the nonlinear dynamical system (3.106) into

$$\frac{d}{dt}(w_i+\delta w_i) \doteq F_i(\mathbf{w}(t)) + \left.\frac{\partial F_i}{\partial w_j}\right|_{\mathbf{w}(t)}\delta w_j \ . \tag{3.114}$$

Eqn. (3.106) then immediately yields

$$\frac{d}{dt}\delta w_i \doteq \left.\frac{\partial F_i}{\partial w_j}\right|_{\mathbf{w}(t)}\delta w_j \ . \tag{3.115}$$

If $\mathbf{w}_0$ is the stationary point, i.e., if $\mathbf{w}(t)=\mathbf{w}_0$, we can write the solution of (3.115) in the form

$$\delta\mathbf{w} = e^{\mathcal{G}(\mathbf{w}_0)t}\delta\mathbf{w}_0 \ , \tag{3.116}$$

where

$$\mathcal{G}_{ij}(\mathbf{w}) = \left.\frac{\partial F_i}{\partial w_j}\right|_{\mathbf{w}} \ , \quad \exp(\mathcal{G}t) = \sum_{n=0}^{\infty}\frac{1}{n!}(\mathcal{G}t)^n \ , \tag{3.117}$$

and hence the exponential growth or damping is characterized by the real parts of the eigenvalues of the matrix $\mathcal{G}$. Remember that we already constructed the matrix $\mathcal{G}$ for the stationary point corresponding to purely conducting state in Section 3.1.7.

The alternative definition of the Lyapunov exponents stems from phase-space volumetric considerations: The equation

$$\delta\mathbf{w}_0\cdot\delta\mathbf{w}_0 = \epsilon^2 \tag{3.118}$$

describes an initial ball in the phase-space with the radius ϵ. Putting (3.112) into (3.118) gives

$$\Pi^{-1}_{ik}(t;\mathbf{w}_0)\Pi^{-1}_{il}(t;\mathbf{w}_0)\delta w_k(t)\delta w_l(t) = \epsilon^2 \ , \tag{3.119}$$

which is the equation of an ellipsoid. If d_i^2 are the eigenvalues of the symmetric matrix $\boldsymbol{\Pi} \cdot \boldsymbol{\Pi}^T$, where ^{T} denotes the transposition, the lengths of the ellipsoid axes are $|d_i|$. Therefore, we may define Lyapunov exponents alternatively by the relation

$$\boxed{\ell_i = \lim_{t \to \infty} \sup \tfrac{1}{t} \ln |d_i(t)|} \,. \tag{3.120}$$

As one can see from the exponential growth of the solution variations, the Lyapunov exponents can serve as a tool for quantifying the chaoticity of the studied dynamical system. Note that for a symmetric propagator matrix both definitions of the Lyapunov exponents would be identical. However, this is not the case of realistic systems, like those studied in thermal convection.

Chapter 4

Mass and momentum equation for mantle convection

Now we will deal in detail with the mass and momentum equations. We will formulate them in a variational form and apply this general approach to both Newtonian and power-law rheologies, which are advocated by rheological experiments with mantle minerals. The variational approach leads to a minimization of corresponding energy functionals expressed in terms of velocities. The existence and uniqueness of the solution will be proved and general gradient optimization techniques prior to discretization will be studied. We will also outline difficulties with the transformation of the nonlinear problem to a series of linear problems and mention the interaction between a domain with the linear creep law and a domain with the nonlinear rheology. There are complications with the determination of pressure after introducing compressibility; we will try to explain them by employing the Lagrange multipliers. To avoid powers of the nabla operator, that appear when the principles are expressed only in terms of velocities, we will formulate also alternative hybrid variational principles, that will be expressed in terms of velocities and stresses. Finally, we will show how to apply the spherical harmonic functions to this problem.

4.1 Variational principles for the Newtonian rheology

In the previous chapters, mantle convection has been studied on the assumption that the momentum equation expresses a balance between the buoyancy force and the deformation force; the inertial force has been neglected. In the case of Newtonian incompressible flow, we have just dealt with the so-called steady-state *Stokes problem* which can be reformulated by means of a variational principle (Temam, 1979). Similar problems of elasticity can also be formulated in variational ways (Nečas & Hlaváček, 1981). From the physical point of view, these variational formulations express fundamental laws of theoretical mechanics. Consequently, the solutions of the variational principles have to satisfy mathematical requirements that are weaker than those for the solutions of corresponding differential equations. The application of modern functional analysis then leads to success in proving the existence, the uniqueness and the stability of the variational solutions, as well as the convergence of optimization techniques designed to achieve them. Moreover, variational formulations naturally serve as the starting points for numerical discretizations of problems by means of basis functions with both local supports (finite elements) and global supports (polynomial series). That is why the study of variational principles used for the momentum equation is of primary importance.

4.1.1 Basic equations

The viscous flow in the mantle is governed by the principles of mass and momentum conservation, which will be considered in the form,

$$\nabla \cdot \boldsymbol{v} = 0 \ , \tag{4.1}$$

$$\nabla \cdot \boldsymbol{\tau} + \boldsymbol{f} = 0 \ , \tag{4.2}$$

where $\boldsymbol{v}$ is the velocity, $\boldsymbol{\tau}$ is the stress tensor and $\boldsymbol{f}$ is the body force induced by density heterogeneities. It is necessary to add a constitutive law describing the rheological behaviour of the mantle material. Here we will consider it in the form

$$\boldsymbol{\tau} = -p\boldsymbol{I} + \boldsymbol{\sigma}(\dot{\boldsymbol{e}}) \ , \tag{4.3}$$

where $p = -\frac{1}{3}Tr(\boldsymbol{\tau})$ is the pressure, $\boldsymbol{I}$ is the identity tensor, $\boldsymbol{\sigma}$ is the deviatoric part of the stress tensor and $\dot{\boldsymbol{e}} = \frac{1}{2}(\nabla\boldsymbol{v} + (\nabla\boldsymbol{v})^T)$ is the strain-rate tensor.

The mantle boundaries are usually considered *impermeable*, i.e.

$$\boldsymbol{v} \cdot \boldsymbol{n} = 0 \tag{4.4}$$

at the boundaries with the unit outer normal denoted by $\boldsymbol{n}$. To complete the boundary conditions, the *free-slip* is considered in the tangential direction:

$$\boldsymbol{\tau} \cdot \boldsymbol{n} - (\boldsymbol{n} \cdot \boldsymbol{\tau} \cdot \boldsymbol{n})\boldsymbol{n} = 0 \ . \tag{4.5}$$

Alternatives to the system (4.4), (4.5), common in geophysical problems, are either *no-slip*

$$\boldsymbol{v} = 0 \tag{4.6}$$

or *stress-free*

$$\boldsymbol{\tau} \cdot \boldsymbol{n} = 0 \tag{4.7}$$

boundary conditions.

4.1.2 Introductory concepts and motivation

We start with a Newtonian flow which is characterized by the linear dependence of the deviatoric stress on the velocity: $\boldsymbol{\sigma}(\dot{\boldsymbol{e}}) = 2\eta\dot{\boldsymbol{e}}$, where the viscosity η, $\eta_1 \geq \eta \geq \eta_0 > 0$, is a 3-D function of spatial variables and $\eta_0 \leq \eta_1$ are constants. We use this rheology to demonstrate basic principles of variational approaches to the problem formulated in the previous subsection.

Introduce the functional

$$F(\boldsymbol{v}) = \int_G \eta(\dot{\boldsymbol{e}} : \dot{\boldsymbol{e}})\, dV - \int_G \boldsymbol{f} \cdot \boldsymbol{v}\, dV \ , \tag{4.8}$$

where G is the domain under study and the symbol ":" denotes again the total scalar product of tensors, i.e. $\dot{\boldsymbol{e}} : \dot{\boldsymbol{e}} = \dot{e}_{ij}\dot{e}_{ij}$ in Cartesian coordinates. The physical meaning of the functional is clear: the first term expresses one half of the dissipative energy and the second term is the power of the body forces. The variation of F considered in the Gâteaux sense,

$$\delta F(\boldsymbol{v}; \delta\boldsymbol{v}) \equiv \frac{\mathrm{d}}{\mathrm{d}t} F(\boldsymbol{v} + t\delta\boldsymbol{v})\bigg|_{t=0} \ ,$$

reads

$$\delta F(\boldsymbol{v}; \delta\boldsymbol{v}) = 2\int_G \eta(\dot{\boldsymbol{e}} : \delta\dot{\boldsymbol{e}})\, dV - \int_G \boldsymbol{f} \cdot \delta\boldsymbol{v}\, dV \ , \tag{4.9}$$

where $\delta\dot{\boldsymbol{e}} = \frac{1}{2}(\nabla\delta\boldsymbol{v} + (\nabla\delta\boldsymbol{v})^T)$. The symmetry of $\dot{\boldsymbol{e}}$ and the Green theorem yield

$$\delta F(\boldsymbol{v}; \delta\boldsymbol{v}) = \int_{\partial G} 2\eta(\boldsymbol{n} \cdot \dot{\boldsymbol{e}} \cdot \delta\boldsymbol{v})\, dS - \int_G [\nabla \cdot (2\eta\dot{\boldsymbol{e}})] \cdot \delta\boldsymbol{v}\, dV - \int_G \boldsymbol{f} \cdot \delta\boldsymbol{v}\, dV \ , \tag{4.10}$$

where ∂G is the boundary of G.

Now we shall deal with the minimization of F constrained on sets X_k, given by the kernels of linear operators $\mathcal{L}_1 : \boldsymbol{v} \mapsto \nabla \cdot \boldsymbol{v}$, $\mathcal{L}_2 : \boldsymbol{v} \mapsto \boldsymbol{v} \cdot \boldsymbol{n}|_{\partial G}$, and $\mathcal{L}_3 : \boldsymbol{v} \mapsto \boldsymbol{v}|_{\partial G}$:

$$X_k = \{\boldsymbol{v};\ \mathcal{L}_1(\boldsymbol{v}) = 0 \ \text{ and } \ \mathcal{L}_k(\boldsymbol{v}) = 0\} = Ker\,(\mathcal{L}_1) \cap Ker\,(\mathcal{L}_k) \ , \quad k = 1, 2, 3 \ . \tag{4.11}$$

To minimize F on X_k, only $\boldsymbol{v} \in X_k$ are taken into account in the definition (4.8) of $F(\boldsymbol{v})$, and the equation

$$\delta F(\boldsymbol{v}; \delta\boldsymbol{v}) = 0 \ \ \forall\, \delta\boldsymbol{v} \in X_k \ , \quad k = 1, 2, 3 \ , \tag{4.12}$$

is solved. This constrained minimization can be converted onto an unconstrained minimization by means of the Lagrange multiplier method, which will help us with the interpretation of eqn. (4.12). The method is based on introducing the functional

$$F_L(\boldsymbol{v}, \lambda, \nu, \boldsymbol{\mu}) = F(\boldsymbol{v}) + \int_G \lambda\nabla \cdot \boldsymbol{v}\, dV + \delta_{2k}\int_{\partial G} \nu\boldsymbol{n} \cdot \boldsymbol{v}\, dS + \delta_{3k}\int_{\partial G} \boldsymbol{\mu} \cdot \boldsymbol{v}\, dS \ , \tag{4.13}$$

where δ_{ij} is the Kronecker δ-matrix. The equation

$$\delta F_L(\boldsymbol{v}, \lambda, \nu, \boldsymbol{\mu}; \delta\boldsymbol{v}, \delta\lambda, \delta\nu, \delta\boldsymbol{\mu}) = 0 \ \ \forall\, (\delta\boldsymbol{v}, \delta\lambda, \delta\nu, \delta\boldsymbol{\mu}) \tag{4.14}$$

is then equivalent to (4.12) but the solution represents the saddle-point since F_L is linear with respect to the Lagrange multipliers λ, ν and $\boldsymbol{\mu}$.

Since

$$\delta F_L(\boldsymbol{v},\lambda,\nu,\boldsymbol{\mu};\delta\boldsymbol{v},\delta\lambda,\delta\nu,\delta\boldsymbol{\mu}) = \delta F(\boldsymbol{v};\delta\boldsymbol{v}) + \int_{\partial G}\lambda\boldsymbol{n}\cdot\delta\boldsymbol{v}\,dS - \int_G \nabla\lambda\cdot\delta\boldsymbol{v}\,dV + \int_G \delta\lambda\nabla\cdot\boldsymbol{v}\,dV +$$

$$\delta_{2k}\int_{\partial G}\nu\boldsymbol{n}\cdot\delta\boldsymbol{v}\,dS + \delta_{2k}\int_{\partial G}\delta\nu\boldsymbol{n}\cdot\boldsymbol{v}\,dS + \delta_{3k}\int_{\partial G}\boldsymbol{\mu}\cdot\delta\boldsymbol{v}\,dS + \delta_{3k}\int_{\partial G}\delta\boldsymbol{\mu}\cdot\boldsymbol{v}\,dS \qquad (4.15)$$

it is clear from (4.10)–(4.14) that the case $k = 3$ corresponds to the system (4.1)–(4.3), (4.6) with $\lambda = -p$, $\boldsymbol{\mu} = -\boldsymbol{\tau}\cdot\boldsymbol{n}|_{\partial G}$. The kernel of the mapping $\boldsymbol{v} \mapsto \dot{\boldsymbol{e}}$ consists of rigid body translations and rotations (Nečas & Hlaváček, 1981) and thus the linear mapping $X_3 \mapsto \dot{\boldsymbol{e}}(\boldsymbol{v})$ is injective, i.e. $Ker\,(\dot{\boldsymbol{e}}) \cap X_3 = 0$. Analogously, if $k = 2$, eqn. (4.12) is equivalent to the system (4.1)–(4.5) with $\nu = -\boldsymbol{\tau}\cdot\boldsymbol{n}\cdot\boldsymbol{n}$ but $Ker\,(\dot{\boldsymbol{e}}) \cap X_2$ is non-zero (if G is a spherical shell, $Ker\,(\dot{\boldsymbol{e}})$ consists of functions describing the rigid-body rotation). Finally, if $k = 1$, eqn. (4.12) is equivalent to the system (4.1)–(4.3), (4.7) and $Ker\,(\dot{\boldsymbol{e}})\cap X_1$ consists of rigid-body translations and rotations for an arbitrary geometry of G. In all cases solutions exist only if

$$\int_G \boldsymbol{f}\cdot\delta\boldsymbol{v}\,dV = 0 \quad \forall\,\delta\boldsymbol{v} \in Ker\,(\dot{\boldsymbol{e}})\ . \qquad (4.16)$$

Otherwise there is no solution of (4.12).

4.1.3 Functional spaces, existence of the solution and gradient searching with projection

Start with general optimization considerations as summarized in the next theorem (see e.g. Nečas & Hlaváček, 1981):

Let H be a Hilbert space with a scalar product (,) and the norm $\|u\| = \sqrt{(u,u)}$ and let X be a linear subspace of H. Let Φ be a functional differentiable in the Gâteaux sense, i.e. $\delta\Phi(u;\delta u) \equiv \frac{\mathrm{d}}{\mathrm{d}t}\Phi(u+t\delta u)\big|_{t=0}$ exists $\forall u \in H,$ and $\forall \delta u \in H$. Suppose that the differential is strongly monotone on H, i.e.,

$$\exists c_1 > 0,\quad \delta\Phi(u+\delta u;\delta u) - \delta\Phi(u;\delta u) \geq c_1\|\delta u\|^2,\quad \forall u \in H, \forall \delta u \in H \qquad (4.17)$$

and Lipschitz continuous on H, i.e.,

$$\exists c_2 > 0,\quad |\delta\Phi(u+\delta u;\delta w) - \delta\Phi(u;\delta w)| \leq c_2\|\delta u\|\|\delta w\| \quad \forall u \in H,\ \forall \delta u \in H, \forall \delta w \in H\ . \qquad (4.18)$$

Then there is a unique $u_m \in X$ that minimizes Φ on X, i.e. $\Phi(u) > \Phi(u_m)\ \forall u \in X,\ u \neq u_m$.

Introduce $\nabla\Phi(u) \in H$ by the relation,

$$\delta\Phi(u;\delta u) = (\nabla\Phi(u), \delta u) \ \ \forall \delta u \in H \tag{4.19}$$

and the projection operator $u \in H \mapsto P(u) \in X$ as usual,

$$(u - P(u), w - P(u)) = 0 \ \ \forall w \in X \ . \tag{4.20}$$

The following fundamental theorem (Nečas & Hlaváček, 1981) shows that the minimum of functionals with the strongly monotone and Lipschitz continuous variation can be found by means of the gradient searching with projection:

Let the variation $\delta\Phi$ be strongly monotone and Lipschitz continuous and let $u^0 \in X$ be arbitrary. Then the limit of the iterations

$$u^{i+1} = P(u^i - \gamma\nabla\Phi(u^i)) \ \ \gamma \in (0, 2c_1/c_2^2) \tag{4.21}$$

exists and is equal to u_m that minimizes Φ on X.

Now go back to the functional F defined by (4.8). To be able to deal with the mathematical properties of the minimization of F, we have to define the functional space of velocities to satisfy an existence of integrals in the definition of F. Let $L^2(G)$ be the space of square integrable functions on G and $\boldsymbol{W}^{1,2}(G)$ the Sobolev space defined by

$$\boldsymbol{W}^{1,2}(G) = \left\{ \boldsymbol{v}; \ v_i \in L^2(G), \ \frac{\partial v_i}{\partial x_j} \in L^2(G) \ \forall i,j \right\} \tag{4.22}$$

with the scalar product

$$(\boldsymbol{v}_1, \boldsymbol{v}_2) = \int_G \boldsymbol{v}_1 \cdot \boldsymbol{v}_2 \, dV + \int_G \nabla\boldsymbol{v}_1 : \nabla\boldsymbol{v}_2 \, dV \tag{4.23}$$

and let the velocities be confined to this space. Then

$$\delta F(\boldsymbol{v} + \delta\boldsymbol{v}; \delta\boldsymbol{w}) - \delta F(\boldsymbol{v}; \delta\boldsymbol{w}) = 2\int_G \eta\delta\dot{\boldsymbol{e}}(\boldsymbol{v}) : \delta\dot{\boldsymbol{e}}(\boldsymbol{w}) \, dV \tag{4.24}$$

and the Lipschitz continuity is clear. According to the so-called Korn's inequality (Nečas & Hlaváček, 1981) there exists $c > 0$ such that

$$\delta F(\boldsymbol{v} + \delta\boldsymbol{v}; \delta\boldsymbol{v}) - \delta F(\boldsymbol{v}; \delta\boldsymbol{v}) = 2\int_G \eta\delta\dot{\boldsymbol{e}}(\boldsymbol{v}) : \delta\dot{\boldsymbol{e}}(\boldsymbol{v}) \, dV \geq$$

$$2\eta_0 \int_G \delta\dot{\boldsymbol{e}}(\boldsymbol{v}) : \delta\dot{\boldsymbol{e}}(\boldsymbol{v}) \, dV \geq c\|\delta\boldsymbol{v}\|^2_{W^{1,2}} \ \forall \delta\boldsymbol{v} \in \boldsymbol{W}^{1,2}(G) \ominus Ker\,(\dot{\boldsymbol{e}}) \ , \tag{4.25}$$

where $\ominus$ denotes the linear subtraction of spaces. The solution of (4.12) is therefore unique if $X = X_3$. In the two other cases, $X = X_1$ and $X = X_2$, the solutions exist and are unique except for the kernels of the operators $X \mapsto \dot{\boldsymbol{e}}$ if and only if (4.16) is satisfied.

Remark:
The question arises how to obtain the pressure and the surface traction if we employ the gradient method with projection to minimize F. According to (4.14) the Lagrange multipliers are determined by the linear problem

$$\delta F_L(\boldsymbol{v}_m, \lambda, \nu, \boldsymbol{\mu}; \delta \boldsymbol{v}) = 0 \quad \forall\, \delta \boldsymbol{v} \ , \tag{4.26}$$

where the multipliers are considered in corresponding L^2-spaces and where the left-hand side denotes the partial variation of F_L with respect to $\boldsymbol{v}$. The linear problem (4.26) is, however, singular as the equation is identically fulfilled for $\delta \boldsymbol{v} \in X_k$. Let $\boldsymbol{\psi} \in \boldsymbol{W}^{1,2}$. Since for $\varphi \in W^{1,2}(G)$

$$\int_G \nabla\varphi \cdot \boldsymbol{\psi}\, dV = \int_{\partial G} \varphi \boldsymbol{\psi} \cdot \boldsymbol{n}\, dS - \int_G \varphi \nabla \cdot \boldsymbol{\psi}\, dV \tag{4.27}$$

and for $\boldsymbol{\varphi} \in \boldsymbol{W}^{1,2}(G)$

$$\int_G (\nabla \times \boldsymbol{\varphi}) \cdot \boldsymbol{\psi}\, dV = \int_{\partial G} \boldsymbol{\varphi} \cdot (\boldsymbol{\psi} \times \boldsymbol{n})\, dS + \int_G \boldsymbol{\varphi} \cdot (\nabla \times \boldsymbol{\psi})\, dV \ , \tag{4.28}$$

where $\times$ denotes the vector product, it is possible to prove that the orthogonal complements of X_k with respect to L_2-norms in the cases $k = 1$ and $k = 2$ are

$$X_1^{\perp} = \{\boldsymbol{w};\ \boldsymbol{w} = \nabla\phi;\ \phi \in W^{2,2}(G);\ \nabla\phi \times \boldsymbol{n}|_{\partial G} = 0\} \ , \quad X_2^{\perp} = \{\boldsymbol{w};\ \boldsymbol{w} = \nabla\phi;\ \phi \in W^{2,2}(G)\} \tag{4.29}$$

(Neittaanmäki & Křížek, 1984; Křížek & Neittaanmäki, 1985). The singularity of (4.26) mentioned above can be removed by confining $\delta \boldsymbol{v}$ to the spaces $X_k^{\perp}$ because they are linearly independent on X_k.

4.1.4 Application of Uzawa's algorithm

An alternative approach to the constrained minimization described above is the direct search for the saddle-point defined by (4.14). Let the partial gradient with respect to the multipliers $\nabla_{(\lambda,\nu,\mu)} F_L(\boldsymbol{v})$ be defined as usual:

$$\delta F_L(\boldsymbol{v}; \delta\lambda, \delta\nu, \delta\boldsymbol{\mu}) = (\nabla_{(\lambda,\nu,\mu)} F_L(\boldsymbol{v}), (\delta\lambda, \delta\nu, \delta\boldsymbol{\mu}))\ \forall (\delta\lambda, \delta\nu, \delta\boldsymbol{\mu}) \ , \tag{4.30}$$

where the right-hand side of (4.30) means the scalar product in the corresponding L_2-spaces of the multipliers. Since the dependence of F_L on the multipliers is linear, the partial variation with respect to the multipliers depends only on the velocity. Knowing some approximation $(\lambda_n, \nu_n, \boldsymbol{\mu}_n)$ of the multipliers, we obtain the corresponding $\boldsymbol{v}_n$ from the equation

$$\delta F_L(\boldsymbol{v}_n, \lambda_n, \nu_n, \boldsymbol{\mu}_n; \delta \boldsymbol{v}) = 0\ \forall \delta \boldsymbol{v} \ , \tag{4.31}$$

which is equivalent to minimizing $F_L(\boldsymbol{v}, \lambda_n, \nu_n, \boldsymbol{\mu}_n)$ with respect to $\boldsymbol{v}$. Now making short steps

$$(\lambda_{n+1}, \nu_{n+1}, \boldsymbol{\mu}_{n+1}) = (\lambda_n, \nu_n, \boldsymbol{\mu}_n) + \alpha_n \nabla_{(\lambda,\nu,\mu)} F_L(\boldsymbol{v}_n) \ , \tag{4.32}$$

with $\alpha_n > 0$ being small enough, we arrive at the iteration procedure which is a special application of the so-called Uzawa algorithm (Nečas & Hlaváček, 1981).

4.1.5 Ritz-Galerkin approximation of the projection operator

In this paragraph we will first remember how to construct finite-dimensional subspaces $H_n \subset H$ and $X_n \subset X$ to achieve the convergence of the "discrete solutions" minimizing Φ on X_n to the solution of the original problem. Secondly, we will deal with the construction of the projection operator in "discrete problems" to be able to employ the projection method.

Let $H_n \subset H$ be finite-dimensional subspaces, $H_n \to H$ in the following sense: For any $u \in H$ there exist $u_n \in H_n$ such that $u_n \to u$. Suppose that X_n are subspaces in H_n and that:
(i) for any $u \in X$ there exist $u_n \in X_n$ such that $u_n \to u$,
(ii) if $w_n \in X_n$ and $w_n \rightharpoonup w$ then $w \in X$ ($\rightharpoonup$ denotes the weak convergence).
Suppose that Φ satisfies (4.17), (4.18). Denote by $v_n \in X_n$ solutions of the problem $\min_{v \in X_n} \Phi(v) = \Phi(v_n)$. Then $v_n \to v_m$, where v_m solves the problem $\min_{v \in X} \Phi(v) = \Phi(v_m)$ (Nečas & Hlaváček, 1981).

Let $\{\psi_i\}_{i=1}^n$ is the set of basis functions of H_n. Using Einstein's summation rule we can write

$$\delta\alpha_j(\nabla\Phi(\alpha_i\psi_i),\psi_j) = (\nabla\Phi(\alpha_i\psi_i),\delta\alpha_j\psi_j) = \frac{\mathrm{d}}{\mathrm{d}t}\Phi(\alpha_i\psi_i + t\delta\alpha_j\psi_j)\bigg|_{t=0} = \frac{\partial\Phi}{\partial\alpha_j}\bigg|_{\alpha_i\psi_i}\delta\alpha_j \ . \tag{4.33}$$

This means that

$$(\nabla\Phi(\alpha_i\psi_i),\psi_j) = \frac{\partial\Phi}{\partial\alpha_j}\bigg|_{\alpha_i\psi_i} \tag{4.34}$$

which yields the components of $\nabla\Phi$:

$$(\nabla\Phi)_m(\alpha_i\psi_i) = (\mathbf{A}^{-1})_{mj}\frac{\partial\Phi}{\partial\alpha_j}\bigg|_{\alpha_i\psi_i} \ , \quad A_{mj} = (\psi_m,\psi_j) \ . \tag{4.35}$$

Let the subspace X_n be generated by means of the linear constraints

$$B_{ij}\alpha_j = 0 \ , \quad i = 1,2,...,l < n \ . \tag{4.36}$$

Employing the definition (4.20), it is easy to show that the projection matrix is then given by

$$\mathbf{P} = \mathbf{E} - \mathbf{A}^{-1}\mathbf{B}^T(\mathbf{B}\mathbf{A}^{-1}\mathbf{B}^T)^{-1}\mathbf{B} \ , \tag{4.37}$$

where $\mathbf{E}$ is the identity matrix. The relations (4.35–4.37) show that the gradient and the projection do not depend only on the choice of the basis $\{\psi_i\}_{i=1}^n$ but they depend also on the choice of the scalar product.

4.2 Variational principles for the power-law rheology

4.2.1 Basic functionals and their peoperties

The real rheology of the Earth is probably governed by a nonlinear power-law under a wide range of temperatures and pressures. The aim of this study is to show that the application of realistic rheologies does not complicate the variational formulations by themselves but that it may lead to some mathematical problems while seeking solutions. To overcome these problems, the power-law rheological relationship should be slightly modified as demonstrated below: we can use, e.g., a composite power-law and Newtonian rheology or the Carreau rheology.

The power-law rheology can be characterized by the following relationship,

$$\dot{\boldsymbol{e}} = A(\boldsymbol{\sigma} : \boldsymbol{\sigma})^{(n-1)/2}\boldsymbol{\sigma} \ , \quad n > 0 \ , \tag{4.38}$$

where A will be considered as a function of spatial variables with its values limited by two constants $0 < A_0 \leq A_1$, i.e., $A_1 \geq A \geq A_0 > 0$, and n is a material parameter. The Newtonian flow is characterized by $n = 1$. Denote $\dot{\boldsymbol{e}}_s \equiv (\dot{\boldsymbol{e}} : \dot{\boldsymbol{e}})^{1/2}$, $\boldsymbol{\sigma}_s \equiv (\boldsymbol{\sigma} : \boldsymbol{\sigma})^{1/2}$. As $\dot{\boldsymbol{e}}_s = A\boldsymbol{\sigma}_s^n$, the inverse relation to (4.38) is

$$\boldsymbol{\sigma} = A^{-1/n}(\dot{\boldsymbol{e}} : \dot{\boldsymbol{e}})^{(1-n)/2n}\dot{\boldsymbol{e}} \ . \tag{4.39}$$

Eq. (4.39) will be employed now to construct the analogy to the functional in (4.8). Since the first integral in (4.8) expresses the half of the rate of the dissipative energy with its volumetric density $\boldsymbol{\sigma} : \dot{\boldsymbol{e}}$, we will deal with the generalization of (4.8) in the form:

$$F(\boldsymbol{v}) = \int_G \frac{n}{n+1} \frac{(\dot{\boldsymbol{e}} : \dot{\boldsymbol{e}})^{(n+1)/2n}}{A^{1/n}} \, dV - \int_G \boldsymbol{f} \cdot \boldsymbol{v} \, dV \ . \tag{4.40}$$

Then the analogy of (4.9) is

$$\delta F(\boldsymbol{v}; \delta\boldsymbol{v}) = \int_G A^{-1/n}(\dot{\boldsymbol{e}} : \dot{\boldsymbol{e}})^{(1-n)/2n}(\dot{\boldsymbol{e}} : \delta\dot{\boldsymbol{e}}) \, dV - \int_G \boldsymbol{f} \cdot \delta\boldsymbol{v} \, dV \tag{4.41}$$

and the analogy of (4.10) is

$$\delta F(\boldsymbol{v}; \delta\boldsymbol{v}) = \int_{\partial G} A^{-1/n}(\dot{\boldsymbol{e}} : \dot{\boldsymbol{e}})^{(1-n)/2n}(\boldsymbol{n} \cdot \dot{\boldsymbol{e}} \cdot \delta\boldsymbol{v}) \, dS - \int_G [\nabla \cdot (A^{-1/n}(\dot{\boldsymbol{e}} : \dot{\boldsymbol{e}})^{(1-n)/2n}\dot{\boldsymbol{e}})] \cdot \delta\boldsymbol{v} \, dV - \int_G \boldsymbol{f} \cdot \delta\boldsymbol{v} \, dV \ . \tag{4.42}$$

To ensure an existence of integrals in F defined by (4.40), introduce the space

$$M(G) = \left\{ \boldsymbol{v}; \ v_i \in L^2(G), \ \frac{\partial v_i}{\partial x_j} \in L^{\frac{n+1}{n}}(G) \right\} \tag{4.43}$$

with the norm

$$\|\boldsymbol{v}\|_M = \left(\int_G \boldsymbol{v}\cdot\boldsymbol{v}\, dV\right)^{\frac{1}{2}} + \left(\int_G (\dot{\boldsymbol{e}} : \dot{\boldsymbol{e}})^{(n+1)/2n}\right)^{\frac{n}{n+1}} \ . \tag{4.44}$$

By Kondrashov embedding theorem (Ciarlet, 1978), $M(G)$ is equal to the Sobolev space $\boldsymbol{W}^{1,(n+1)/n}(G)$ for $n > \frac{1}{2}$.

It is easy to show that δF is not strongly monotone on $M(G)$ if $n \neq 1$. In general,

$$\delta F(\boldsymbol{v}+\delta\boldsymbol{v};\delta\boldsymbol{v}) - \delta F(\boldsymbol{v};\delta\boldsymbol{v}) =$$

$$\int_G A^{-1/n}((\dot{\boldsymbol{e}}+\delta\dot{\boldsymbol{e}}) : (\dot{\boldsymbol{e}}+\delta\dot{\boldsymbol{e}}))^{(1-n)/2n}(\dot{\boldsymbol{e}}+\delta\dot{\boldsymbol{e}}) : (\delta\dot{\boldsymbol{e}})\, dV - \int_G A^{-1/n}(\dot{\boldsymbol{e}} : \dot{\boldsymbol{e}})^{(1-n)/2n}(\dot{\boldsymbol{e}} : \delta\dot{\boldsymbol{e}})\, dV \ . \tag{4.45}$$

We now examine now the properties of the mapping $\delta\boldsymbol{v} \mapsto \delta F(\boldsymbol{0},\delta\boldsymbol{v})$:
Let ϵ be a positive constant. Then

$$\delta F(\epsilon\delta\boldsymbol{v};\epsilon\delta\boldsymbol{v}) - \delta F(0;\epsilon\delta\boldsymbol{v}) = \int_G A^{-1/n}(\epsilon\delta\dot{\boldsymbol{e}} : \epsilon\delta\dot{\boldsymbol{e}})^{(1+n)/2n}\, dV \leq \epsilon^{(1+n)/n} A_0^{-1/n}\|\delta\boldsymbol{v}\|_M^{(1+n)/n} \ . \tag{4.46}$$

Let $c > 0$ be an arbitrary constant and $\delta\boldsymbol{v} \neq 0$ fixed. If $0 < n < 1$ there exists ϵ small enough such that

$$\epsilon^{(1+n)/n} A_0^{-1/n}\|\delta\boldsymbol{v}\|_M^{(1+n)/n} < c\,\epsilon^2\|\delta\boldsymbol{v}\|_M^2 = c\|\epsilon\delta\boldsymbol{v}\|_M^2 \ . \tag{4.47}$$

On the other hand, if $n > 1$ then there exists ϵ large enough such that (4.47) again holds. In the both cases we have thus found the situation when the strong monotonicity is broken.

To study the problem of strong monotonicity more deeply, let us deal with

$$\delta^2 F(\boldsymbol{v};\delta\boldsymbol{v},\delta\boldsymbol{w}) = \frac{\mathrm{d}}{\mathrm{d}t}\delta F(\boldsymbol{v}+t\delta\boldsymbol{w};\delta\boldsymbol{v})\bigg|_{t=0} \ .$$

We have

$$\delta^2 F(\boldsymbol{v};\delta\boldsymbol{v},\delta\boldsymbol{v}) = \int_G \frac{1-n}{nA^n}(\dot{\boldsymbol{e}} : \dot{\boldsymbol{e}})^{(1-3n)/2n}(\dot{\boldsymbol{e}} : \delta\dot{\boldsymbol{e}})(\dot{\boldsymbol{e}} : \delta\dot{\boldsymbol{e}})\, dV +$$
$$\int_G A^{-1/n}(\dot{\boldsymbol{e}} : \dot{\boldsymbol{e}})^{(1-n)/2n}(\delta\dot{\boldsymbol{e}} : \delta\dot{\boldsymbol{e}})\, dV \ . \tag{4.48}$$

According to the Schwarz inequality

$$(\dot{\boldsymbol{e}} : \delta\dot{\boldsymbol{e}})(\dot{\boldsymbol{e}} : \delta\dot{\boldsymbol{e}}) \leq (\dot{\boldsymbol{e}} : \dot{\boldsymbol{e}})(\delta\dot{\boldsymbol{e}} : \delta\dot{\boldsymbol{e}}) \ . \tag{4.49}$$

Since $\frac{1-n}{n} > -1$ for $n > 0$, $\delta^2 F(\boldsymbol{v};\delta\boldsymbol{v},\delta\boldsymbol{v}) > 0$ if $\dot{\boldsymbol{e}}(\boldsymbol{v}) \neq 0$ almost everywhere, as follows from (4.48) and (4.49). Therefore $\delta F(\boldsymbol{v};\delta\boldsymbol{v})$ is not strongly monotone only if there is a subdomain of G, where the strain is zero.

Nevertheless, the problem of uniqueness of the solution can be solved by means of the convex analysis:
Let $t \in (0,1)$, $n > 0$ and $\dot{\boldsymbol{e}}^{(1)} \neq \dot{\boldsymbol{e}}^{(2)}$ be two strains. Then

$$\left[(\dot{\boldsymbol{e}}^{(1)} + t(\dot{\boldsymbol{e}}^{(2)} - \dot{\boldsymbol{e}}^{(1)})) : (\dot{\boldsymbol{e}}^{(1)} + t(\dot{\boldsymbol{e}}^{(2)} - \dot{\boldsymbol{e}}^{(1)}))\right]^{(n+1)/2n} <$$

$$\left[\dot{\boldsymbol{e}}^{(1)} : \dot{\boldsymbol{e}}^{(1)}\right]^{(n+1)/2n} + t\left[(\dot{\boldsymbol{e}}^{(2)} - \dot{\boldsymbol{e}}^{(1)}) : (\dot{\boldsymbol{e}}^{(2)} - \dot{\boldsymbol{e}}^{(1)})\right]^{(n+1)/2n} \quad . \tag{4.50}$$

This inequality satisfies the mapping $\dot{\boldsymbol{e}} \mapsto F$ to be strongly convex for any $n > 0$ and, therefore, the mapping $\boldsymbol{v} \mapsto F$ is also strongly convex except for $Ker\,(\dot{\boldsymbol{e}})$. Since it is also continuous on M if $f_i \in L^2(G)$, there is one and only one $\boldsymbol{v}_m$ that minimizes F on M except for $Ker\,(\dot{\boldsymbol{e}})$ (Fučík and Kufner, 1980). However, the gradient searching of the solution may fail.

4.2.2 Effective viscosity and transformation of the non-linear problem into a sequence of linear problems

Let us go back to eqn. (4.39). Introducing the so-called effective viscosity

$$\eta(\boldsymbol{v}) = \frac{1}{2} A^{-1/n} (\dot{\boldsymbol{e}} : \dot{\boldsymbol{e}})^{(1-n)/2n} \ , \tag{4.51}$$

we can interpret the basic rheological relationship as that of a Newtonian fluid with velocity-dependent viscosity. Having the q-th approximation $\boldsymbol{v}_q$ of the problem, it is natural to seek $\boldsymbol{v}_{q+1}$ as the solution of the problem for the linear rheology

$$\boldsymbol{\sigma} = 2\eta(\boldsymbol{v}_q)\dot{\boldsymbol{e}} \ , \tag{4.52}$$

which is the basic idea of the method of secant modules. The convergence of the method in its abstract version can be proved for functionals with strongly monotone variation defined on a Hilbert space (Nečas & Hlaváček, 1981). Our functional is not strongly monotone if there is a subdomain of G with zero strain and, moreover, the space $M(G)$ is not a Hilbert space. In general, we are thus not able to prove the convergence of the method for the problems with the power-law rheology. This, of course, does not mean that the method cannot converge at all! The method was used with a great success in mantle dynamics problems. We should,however, be aware of the fact that the application of the method is not universal. To avoid problems with possible zero deformations, i.e., with zero ($0 < n < 1$) or infinite ($n > 1$) effective viscosity, it is possible, e.g., to consider *a composite non-Newtonian and Newtonian rheology*: (van den Berg et al., 1993): if $0 < n < 1$ it is sufficient to assume that the deviatoric stress consists of the two terms, Newtonian and non-Newtonian; if, on the other hand, $n > 1$, it is sufficient to split the strain tensor into analogous terms. The other possibility is to use *the Carreau rheology* which is a generalization of the power-law stress-strain relationship. In such a case the effective viscosity is

$$\eta(\boldsymbol{v}) = \frac{1}{2} A^{-1/n} (\gamma + \dot{\boldsymbol{e}} : \dot{\boldsymbol{e}})^{(1-n)/2n} \ , \tag{4.53}$$

where $\gamma \geq \gamma_0 > 0$ is a function of spatial coordinates — usually considered as a constant.

4.2.3 Interaction between subdomains with different rheology

Up to now we have implicitly assumed that the power n in the basic rheological relationship (4.38) is the same throughout the whole domain G. However, this is not necessary as clear from the variational formulation (4.40). Hence, n may be a function of spatial variables, which corresponds, e.g., to whole mantle problems as the rheology of the upper mantle is probably non-linear but the lower mantle may be Newtonian. This is the special situation because the style of convection in the Newtonian subdomain is a linear function of the inner forces and the conditions on the boundary of the subdomain. After constructing this function, it is possible to confine the problem only to the non-linear part as will be demonstrated below.

Let $G = G_1 \cup G_2 \cup \{\partial G_1 \cap \partial G_2\}$, G_1, G_2 be adjacent, and let $n = 1$ in G_1. We may write

$$F(\boldsymbol{v}) = F_1(\boldsymbol{v}) + F_2(\boldsymbol{v}) \equiv \int_{G_1} \frac{1}{2} \frac{(\dot{\boldsymbol{e}} : \dot{\boldsymbol{e}})}{A}\, dV - \int_{G_1} \boldsymbol{f} \cdot \boldsymbol{v}\, dV + \int_{G_2} \frac{n}{n+1} \frac{(\dot{\boldsymbol{e}} : \dot{\boldsymbol{e}})^{(n+1)/2n}}{A^{1/n}}\, dV - \int_{G_2} \boldsymbol{f} \cdot \boldsymbol{v}\, dV \ , \tag{4.54}$$

where $\boldsymbol{v} \in M(G) \cap X_k$. To be able to split the problem into the minimization of F_1 and F_2 it is necessary to split also the space $M(G)$:

$$M(G) = \left\{ \boldsymbol{v};\ \boldsymbol{v}|_{G_1} \equiv \boldsymbol{v}_1 \in \boldsymbol{W}^{1,2}(G_1),\ \boldsymbol{v}|_{G_2} \equiv \boldsymbol{v}_2 \in M(G_2),\ \boldsymbol{v}_1 = \boldsymbol{v}_2 \text{ on } \delta G_1 \cap \delta G_2 \right\} \ . \tag{4.55}$$

The minimization of $F(\boldsymbol{v})$ is then equivalent to the searching a saddle point of

$$F_s(\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{\mu}) = F_1(\boldsymbol{v}_1) + F_2(\boldsymbol{v}_2) - \int_{\partial G_1 \cap \partial G_2} \boldsymbol{\mu} \cdot (\boldsymbol{v}_1 - \boldsymbol{v}_2)\, dS \ , \tag{4.56}$$

where $\boldsymbol{v}_1 \in \boldsymbol{W}^{1,2}(G_1) \cap X_k$, $\boldsymbol{v}_2 \in M(G_2) \cap X_k$. Taking into account the expressions for performing the variation (4.41) and (4.42), we can see that the multiplier $\boldsymbol{\mu}$ can be interpreted as the boundary force acting between the subdomains G_1 and G_2. Since the rheology in G_1 is linear, it is possible to construct the linear affine mappings $\boldsymbol{\nu} \mapsto \boldsymbol{v}_1$ and $\boldsymbol{\nu} \mapsto \boldsymbol{\mu}$ defined on $\partial G_1 \cap \partial G_2$, where $\boldsymbol{\mu}$ is the force acting again on $\partial G_1 \cap \partial G_2$ and both mappings are the results of the linear problem on G_1 with the boundary condition $\boldsymbol{v}_1 = \boldsymbol{\nu}$ on $\partial G_1 \cap \partial G_2$. After constructing these mappings, the rest of the problem is given by the seeking the critical point of the functional

$$F_{2,1}(\boldsymbol{v}_2, \boldsymbol{\nu}) = F_2(\boldsymbol{v}_2) - \int_{\partial G_1 \cap \partial G_2} \boldsymbol{\mu}(\boldsymbol{\nu}) \cdot (\boldsymbol{\nu} - \boldsymbol{v}_2)\, dS \ , \tag{4.57}$$

where $\boldsymbol{v}_2 \in M(G_2) \cap X_k$.

4.2.4 Materials compressed by a hydrostatic pressure

In geophysical applications, the body force $\boldsymbol{f}$ may be usually split into two parts

$$\boldsymbol{f} = \boldsymbol{f}_0 + \boldsymbol{f}_1 \ , \quad |\boldsymbol{f}_1| \ll |\boldsymbol{f}_0| \ , \tag{4.58}$$

where $\boldsymbol{f}_0$ generates the hydrostatic pressure p_0, i.e.,

$$-\nabla p_0 + \boldsymbol{f}_0 = 0 \ . \tag{4.59}$$

Assume that the mass density distribution in the region under study can be described by a function ρ_0 when only force $\boldsymbol{f}_0$ acts in the system. Neglecting other influences on the changes of density, we may rewrite eqns. (4.1)–(4.3) into the system

$$\nabla \cdot (\rho_0 \boldsymbol{v}) = 0 \ , \tag{4.60}$$

$$\nabla \cdot \boldsymbol{\tau}_1 + \boldsymbol{f}_1 = 0 \ , \tag{4.61}$$

$$\boldsymbol{\tau}_1 = -p_1 \boldsymbol{I} + \boldsymbol{\sigma}(\dot{\boldsymbol{e}}) \ , \quad \dot{\boldsymbol{e}} = \frac{1}{2}(\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T - \frac{2}{3}(\nabla \cdot \boldsymbol{v})\boldsymbol{I}) \ , \tag{4.62}$$

where $p_1 = p - p_0$. Comparing the system (4.60)–(4.62) with (4.1)–(4.3), one can see that the only substantial change consists in replacing the solenoidal field (4.1) by the velocity field (4.60). The substitutions $\boldsymbol{f} \to \boldsymbol{f}_1$, $\boldsymbol{\tau} \to \boldsymbol{\tau}_1$ and $p \to p_1$ are, from the mathematical point of view, only formal. In the definition (4.11) of the spaces X_k the change of the operator $\mathcal{L}_1$ is thus necessary. Its new expression is as follows; $\mathcal{L}_1 : \boldsymbol{v} \mapsto \nabla \cdot (\rho_0 \boldsymbol{v})$, where ρ_0 is considered to be a known function $\rho_{max} \geq \rho_0 \geq \rho_{min} > 0$. Consequently, the meaning of the Lagrange multiplier λ is different and (4.13) must be replaced by

$$F_L(\boldsymbol{v}, \lambda, \nu, \boldsymbol{\mu}) = F(\boldsymbol{v}) + \int_G \lambda \nabla \cdot (\rho_0 \boldsymbol{v}) \, dV + \delta_{2k} \int_{\partial G} \nu \boldsymbol{n} \cdot \boldsymbol{v} \, dS + \delta_{3k} \int_{\partial G} \boldsymbol{\mu} \cdot \boldsymbol{v} \, dS \ , \tag{4.63}$$

After performing δF_L, similarly as in (4.15), it is clear that

$$\nabla p_1 + \rho_0 \nabla \lambda = 0 \quad \text{in } G \ , \tag{4.64}$$

$$p_1 + \rho_0 \lambda = 0 \quad \text{on } \partial G \ . \tag{4.65}$$

The applying of the operator $\nabla \cdot$ to (4.64) yields

$$\nabla^2 p_1 = -\nabla \cdot (\rho_0 \nabla \lambda) \ . \tag{4.66}$$

The equation (4.66) with the boundary condition (4.65) can serve for computing the pressure after the Lagrange multiplier λ was obtained.

4.3 Hybrid variational principles

Up to now, the only variable that has been used to construct the energy functional F has been the velocity. The solution $\boldsymbol{v}_m$ minimizes the energy functional on the chosen set X_k. This enables us to use a variety of optimization techniques to find the solution — in the previous section we demonstrated the possibility of employing the gradient searching with projection. There is, however, a very important problem that arises when F is evaluated numerically: in the case of the power-law rheology, the non-linear term in (4.40) contains the power of the differential operator $\boldsymbol{v} \mapsto \dot{\boldsymbol{e}}$ and its numerical realization for a real n may be complicated. To avoid this problem, we will present here a hybrid principle, where the pressure and the deviatoric stress are additional independent variables. The dissipative energy can then be expressed by means of the deviatoric stress only, and thus $\dot{\boldsymbol{e}}$ disappears from the non-linear term.

The functional we will deal with is

$$H(\boldsymbol{\sigma}, \boldsymbol{v}, p) = \int_G \frac{A}{n+1}(\boldsymbol{\sigma} : \boldsymbol{\sigma})^{(n+1)/2}\, dV - \int_G \dot{\boldsymbol{e}} : (-p\boldsymbol{I} + \boldsymbol{\sigma})\, dV + \int_G \boldsymbol{f} \cdot \boldsymbol{v}\, dV +$$
$$\delta_{2k} \int_{\partial G} \boldsymbol{n}(\boldsymbol{v} \cdot \boldsymbol{n}) \cdot (-p\boldsymbol{I} + \boldsymbol{\sigma}) \cdot \boldsymbol{n}\, dS + \delta_{3k} \int_{\partial G} \boldsymbol{v} \cdot (-p\boldsymbol{I} + \boldsymbol{\sigma}) \cdot \boldsymbol{n}\, dS \ , \tag{4.67}$$

where index k distinguishes boundary conditions as in the previous sections. From the mathematical point of view, it is important that there are no derivatives of the deviatoric stress or of the pressure. On the other hand, the derivatives of the velocity must have a "good meaning" if they are integrated — if $n = 1$, it is sufficient if $p \in L^2(G)$, $D_{ij} \in L^2(G)$ and $v_i \in W^{1,2}(G)$.

The variation of H reads

$$\delta H(\boldsymbol{\sigma}, \boldsymbol{v}, p; \delta\boldsymbol{\sigma}, \delta\boldsymbol{v}, \delta p) = \int_G A(\boldsymbol{\sigma} : \boldsymbol{\sigma})^{(n-1)/2}(\boldsymbol{\sigma} : \delta\boldsymbol{\sigma})\, dV -$$
$$\int_G \dot{\boldsymbol{e}} : (-\delta p\boldsymbol{I} + \delta\boldsymbol{\sigma})\, dV - \int_G \delta\dot{\boldsymbol{e}} : (-p\boldsymbol{I} + \boldsymbol{\sigma})\, dV + \int_G \boldsymbol{f} \cdot \delta\boldsymbol{v}\, dV +$$
$$\delta_{2k} \int_{\partial G} \boldsymbol{n}(\delta\boldsymbol{v} \cdot \boldsymbol{n}) \cdot (-p\boldsymbol{I} + \boldsymbol{\sigma}) \cdot \boldsymbol{n}\, dS + \delta_{2k} \int_{\partial G} \boldsymbol{n}(\boldsymbol{v} \cdot \boldsymbol{n}) \cdot (-\delta p\boldsymbol{I} + \delta\boldsymbol{\sigma}) \cdot \boldsymbol{n}\, dS +$$
$$\delta_{3k} \int_{\partial G} \delta\boldsymbol{v} \cdot (-p\boldsymbol{I} + \boldsymbol{\sigma}) \cdot \boldsymbol{n}\, dS + \delta_{3k} \int_{\partial G} \boldsymbol{v} \cdot (-\delta p\boldsymbol{I} + \delta\boldsymbol{\sigma}) \cdot \boldsymbol{n}\, dS \ . \tag{4.68}$$

The Green theorem yields

$$-\int_G \delta\dot{\boldsymbol{e}} : (-p\boldsymbol{I} + \boldsymbol{\sigma})\, dV = -\int_{\partial G} \delta\boldsymbol{v} \cdot (-p\boldsymbol{I} + \boldsymbol{\sigma}) \cdot \boldsymbol{n}\, dS + \int_G \delta\boldsymbol{v} \cdot (-\nabla p + \nabla \cdot \boldsymbol{\sigma})\, dV \ , \tag{4.69}$$

where we have used the symmetry of $\delta\boldsymbol{\sigma}$. After putting (4.69) into (4.68) one can see that the equation $\delta H = 0$ corresponds to the basic set of equations (4.1)–(4.7): the variation of H with respect to the pressure gives the condition of incompressibility, the variation with respect to the deviatoric stress gives the power-law rheology relationship, the variation with respect to the velocity gives the momentum equation and the variations of boundary integrals imply that the boundary conditions are satisfied.

In the case of compressed flow the expression of H is

$$H(\boldsymbol{\sigma}, \boldsymbol{v}, \lambda) = \int_G \frac{A}{n+1}(\boldsymbol{\sigma} : \boldsymbol{\sigma})^{(n+1)/2}\, dV - \int_G (\nabla(\rho_0\boldsymbol{v}) : \lambda\boldsymbol{I} + \dot{\boldsymbol{e}} : \boldsymbol{\sigma})\, dV + \int_G \boldsymbol{f} \cdot \boldsymbol{v}\, dV +$$
$$\delta_{2k} \int_{\partial G} \boldsymbol{n}(\boldsymbol{v} \cdot \boldsymbol{n}) \cdot (\rho_0\lambda\boldsymbol{I} + \boldsymbol{\sigma}) \cdot \boldsymbol{n}\, dS + \delta_{3k} \int_{\partial G} \boldsymbol{v} \cdot (\rho_0\lambda\boldsymbol{I} + \boldsymbol{\sigma}) \cdot \boldsymbol{n}\, dS \ , \tag{4.70}$$

and the pressure can again be computed from (4.65), (4.66) a posteriori.

Recommended reading:

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