Finite element models of steady state Rayleigh-Benard convection. 2) influence of non-linear rheologies

C. Thieulot

March 28, 2017

1 Introduction

In the first computer practical, we looked at the lassic benchmark suite introduced by Blankenbach et al. [2] to validate thermal convection simulations with constant and weakly temperature-dependent viscosity in a 2-D Cartesian box. Because of its simplicity and despite its agedness, this benchmark has become de facto a standard for the geodynamics community. The "Blankenbach benchmark" is not only continuously used to validate modern convection codes [6] [4] [11][10] but also represents a practical starting point upon which more complex benchmark scenarios can be built, as demonstrated by the series of tests for compressible anelastic convec- tion proposed by King et al [9].

Here we extend this classic benchmark suite by considering a rheological formulation with a viscosity that, besides being temperature and pressure dependent, also depends nonlinearly on the strain rate. In particular, we focus on the role of the yield stress, showing how this parameter, by controlling the viscosity distribution at low temperatures and high stresses, is ultimately responsible for the mode of surface deformation: from mobile lid (corresponding to low values of the yield stress), to episodic mobilization (for intermediate values), to stagnant lid (for large values).

In this second practical, We will therefore run five benchmark cases leading to stagnant lid, mobile lid, and periodic convection in a 2D square box. We will also look at a bifurcation analysis, describing the transition from a mobile lid regime to a periodic regime, and from a periodic regime to a stagnant lid regime, as a function of the yield stress.

The following sections contain descriptions of the numerical model and the experiments to be done.

Mandatory reading: "Mantle convection simulations with rheologies that generate plate-like behaviour", by Trompert and Hansen, Nature 395, 1998.

2 The governing model equations

In this computerlab you will perform experiments with numerical solutions of the coupled equations describing thermal convection in an incompressible viscous fluid with infinite Prandtl number[1].

In what follows, the assumption is made that geological materials can be treated as fluids (with special properties) within the realm of continuum fluid mechanics. A Boussinesq approximation is applied, neglecting density variations in the equations except in the buoyancy term of the momentum conservation equation. We consider two-dimensional problems.

$$\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}+\rho(T)\boldsymbol{g} = \mathbf{0} \tag{1}$$

$$\boldsymbol{\nabla}\cdot\boldsymbol{v} = 0 \tag{2}$$

$$\boldsymbol{\sigma} = -p\mathbf{1}+\boldsymbol{s} \tag{3}$$

$$\boldsymbol{s} = 2\mu\dot{\boldsymbol{\epsilon}} \tag{4}$$

$$\dot{\boldsymbol{\epsilon}} = \frac{1}{2}\left(\boldsymbol{\nabla}\boldsymbol{v}+(\boldsymbol{\nabla}\boldsymbol{v})^T\right) \tag{5}$$

$$\rho_0 c_p\left(\frac{\partial T}{\partial t}+\boldsymbol{v}\cdot\boldsymbol{\nabla}T\right) = \boldsymbol{\nabla}\cdot(k\boldsymbol{\nabla}T) \tag{6}$$

$$\rho(T) = \rho_0(1-\alpha T) \tag{7}$$

Equation (1) is the momentum conservation equation and Eq. (2) is the mass conservation equation for incompressible fluids. One can resolve the stress tensor $\boldsymbol{\sigma}$ into its spherical part $-p\mathbf{1}$ and its stress deviation $\boldsymbol{s}$ (see Eq. (3)), where the deviatoric stress tensor is proportional to the strain rate tensor $\dot{\boldsymbol{\epsilon}}$ (see Eq.(4)) through the dynamic viscosity μ. Finally Eq. (5) relates the strain rate tensor to the velocity field.

[1] In heat transfer problems, the Prandtl number controls the relative thickness of the momentum and thermal boundary layers. When Pr is small, it means that the heat diffuses quickly compared to the velocity (momentum).

symbol	meaning and dimension
$\boldsymbol{g}$	gravity acceleration vector $(m.s^{-2})$
L_x, L_y	domain size (m)
p	pressure (Pa)
$\boldsymbol{s}$	deviatoric stress vector (Pa)
$\boldsymbol{v} = (u, v, w)$	velocity $(m.s^{-1})$
$\dot{\boldsymbol{\epsilon}}$	strain-rate tensor (s^{-1})
λ	penalty coefficient $(Pa.s)$
μ	viscosity $(Pa.s)$
ρ, ρ_0	mass density $(kg.m^{-3})$
$\boldsymbol{\sigma}$	stress tensor (Pa)
k	heat conductivity
c_p	heat capacity
α	thermal expansion

Table 1: Nomenclature

Equations (1), (2), (3), (4) and (5) all together lead to the following form of the Stokes equations:

$$\boldsymbol{\nabla} \cdot [\mu(\boldsymbol{\nabla v} + \boldsymbol{\nabla v}^T)] - \boldsymbol{\nabla} p + \rho \boldsymbol{g} = \boldsymbol{0} \tag{8}$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{v} = 0 \tag{9}$$

Equation (11) is an elliptic equation characterized by the fact that changes in buoyancy and constitutive relationships anywhere in the domain have an immediate influence on the entire domain.

3 Numerical solution of the equations

3.1 The penalty method

In order to impose the incompressibility constraint, we shall use a widely used procedure, namely the the penalty method [1, 8]. It is implemented in the code you are going to use, which allows for the elimination of the pressure variable from the momentum equation (resulting in a reduction of the matrix size). Mathematical details on the origin and validity of the penalty approach applied to the Stokes problem can for instance be found in [3] or [7].

The penalty formulation of the mass conservation equation is based on a relaxation of the incompressibility constraint and writes

$$\boldsymbol{\nabla} \cdot \boldsymbol{v} + \frac{p}{\lambda} = 0 \tag{10}$$

where λ is the penalty parameter, that can be interpreted (and has the same dimension) as a bulk viscosity. It is equivalent to say that the material is weakly compressible. It can be shown that if one chooses λ to be a relatively large number, the continuity equation $\boldsymbol{\nabla} \cdot \boldsymbol{v} = 0$ will be approximately satisfied in the finite element solution. The value of λ is often recommend to be 6 to 7 orders of magnitude larger than the shear viscosity [5, 8].

Eq. (10) can be used to eliminate the pressure in Eq. (11) so that the mass and momentum conservation equations fuse to become :

$$\boldsymbol{\nabla} \cdot [\mu(\boldsymbol{\nabla v} + \boldsymbol{\nabla v}^T)] + \lambda \boldsymbol{\nabla}(\boldsymbol{\nabla} \cdot \boldsymbol{v}) + \rho \boldsymbol{g} = \boldsymbol{0} \tag{11}$$

3.2 The finite element method

Introduced in the late 1950s, the finite element method (FEM) [8, 15] has emerged as one of the most powerful numerical methods so far devised.

Quadrilateral/hexahedral Q_1P_0 elements (bi/tri-linear velocity, piecewise constant pressure) are used in this code. Despite the fact that they violate the Ladyzhenskaya, Babouska and Brezzi (LBB) stability condition [5], they remain a popular practical choice in mixed finite element approximation of incompressible materials.

This popularity can be explained by factors such as a) local mass conservation ; b) simple and uniform data structures and algebraic problems with manageable sizes and small bandwidths. The latter are of paramount importance for problems where geometry resolution requires very fine meshes and higher order elements can quickly lead to intractable algebraic problems in three space dimensions.

The physical domain Ω is broken up into elements, and a set of finite element basis functions is defined for each element so that functional representations of the independent variables can be constructed.

A thorough mathematical treatment of the finite element formulation of the equations gouverning the physics of the system is beyond the scope of this work, and has been exposed rigorously in some key references: the reader

is referred to [5] or [7] for details on the theory and implementation of viscous incompressible flows, and to [12] for details on the theory and implementation of the heat transport equation. The FEM formulation of Eqs. (11) and (6) is presented succinctly in the next section.

Even though Eqs. (11) and (6) are coupled through the viscosity and density dependences on temperature and/or velocity, these equations are traditionally not solved in a coupled manner. The obtention of a new set of variables $(\boldsymbol{v}, p, T)$ at a given time is the product of a three-stage process:

1. solve for velocity field
2. recover pressure field from velocity field
3. solve for temperature

The size of the assembled FE matrix grows like the square of the total number of nodes, but this matrix is very sparse. Contrarily to optimised FE codes, no appropriate sparse storage scheme (lower triangular compressed sparse column, or CSC) is used in the code you are going to use. This strongly limits the number of elements/nodes which a grid can count.

The Galerkin finite element equation corresponding to Eq. (11) is

$$(\boldsymbol{K}_\mu + \boldsymbol{K}_\lambda) \cdot \boldsymbol{v} = \boldsymbol{B}$$

with

$$\boldsymbol{K}_\mu = \int_\Omega \boldsymbol{B}^T \cdot \boldsymbol{D}_\mu \cdot \boldsymbol{B} \; d\Omega$$

$$\boldsymbol{K}_\lambda = \int_\Omega \boldsymbol{B}^T \cdot \boldsymbol{D}_\lambda \cdot \boldsymbol{B} \; d\Omega$$

$$\boldsymbol{B} = \int_\Omega \boldsymbol{N}^T \rho \boldsymbol{g} \; d\Omega$$

$$\boldsymbol{D}_\mu^{2D} = \mu \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \boldsymbol{D}_\lambda^{2D} = \lambda \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and where $\boldsymbol{N}$ is the vector of shape functions, and $\boldsymbol{B}$ is the matrix of spatial derivatives of the shape functions.

The finite element equation corresponding to the heat transfer equation is

$$\boldsymbol{M}_c \cdot \frac{\partial \boldsymbol{T}}{\partial t} + (\boldsymbol{K}_a + \boldsymbol{K}_d) \cdot \boldsymbol{T} = \boldsymbol{F}$$

where

$$\boldsymbol{M}_c = \int_\Omega \boldsymbol{N}^T \rho c_P \boldsymbol{N} \; d\Omega$$

$$\boldsymbol{K}_a = \int_\Omega (\boldsymbol{N}^\star)^T \rho c_P \boldsymbol{v} \cdot \boldsymbol{B} \; d\Omega \tag{12}$$

$$\boldsymbol{K}_d = \int_\Omega \boldsymbol{B}^T k \boldsymbol{B} \; d\Omega$$

$$\boldsymbol{F} = \int_\Omega \boldsymbol{N}^T H \; d\Omega$$

where $\boldsymbol{T}$ is the vector of the nodal temperatures and $\boldsymbol{v}$ is the vector of nodal velocities.

3.3 Non-Newtonian rheologies

The viscosity field μ is calculated as the harmonic average between a linear part μ_{lin} that depends on temperature only or on temperature and depth z (with $z = 1 - y$), and a nonlinear, plastic part μ_{plast} dependent on the strain rate

$$\mu(T, z, \dot{\epsilon}) = 2 \left(\frac{1}{\mu_{lin}(T, z)} + \frac{1}{\mu_{plast}(\dot{\epsilon})} \right)^{-1} \tag{13}$$

The linear part is given by the linearized Arrhenius law (the so-called Frank-Kamenetskii approximation [Frank-Kamenetskii, 1969])

$$\mu_{lin}(T, z) = \exp(-\gamma_T T + \gamma_z z) \tag{14}$$

case	Ra	$\Delta\mu_T$	$\Delta\mu_z$	$\mu^\star$	σ_y	Convective regime
1	10^2	10^5	1			Stagnant lid
2	10^2	10^5	1	10^{-3}	1	Mobile lid
3	10^2	10^5	10			Stagnant lid
4	10^2	10^5	10	10^{-3}	1	Mobile lid
5	10^2	10^5	10	10^{-3}	3-6	Mobile lid-periodic-stagnant lid

Table 2: In Cases 1 and 3, the viscosity is directly calculated from equation 14, while for Cases 2, 4, 5a, and 5b, we used equation 13. For a given mesh resolution, Case 5b requires running simulations with yield stress varying between 3 and 5 (see text for details).

where $\gamma_T = \ln(\Delta\mu_T)$ and $\gamma_z = \ln(\Delta\mu_z)$ are parameters controlling the total viscosity contrast due to temperature and pressure. The nonlinear part is given by [14]

$$\mu_{plast}(\epsilon) = \mu^\star + \frac{\sigma_y}{\sqrt{\dot{\boldsymbol{\epsilon}} : \dot{\boldsymbol{\epsilon}}}} \tag{15}$$

where $\mu^\star$ is a constant representing the effective viscosity at high stresses [13] and σ_y is the yield stress, also assumed to be constant. In 2D, the denominator is given explicitly by

$$\sqrt{\dot{\boldsymbol{\epsilon}} : \dot{\boldsymbol{\epsilon}}} = \sqrt{\dot{\epsilon}_{ij}\dot{\epsilon}_{ij}}$$

The viscoplastic flow law (equation 13) leads to linear viscous deformation at low stresses (equation 14) and to plastic deformation for stresses that exceed σ_y (equation 15), with the decrease in viscosity limited by the choice of $\mu^\star$ [13]. for a discussion of the combined role of $\mu^\star$ and σ_y on the resulting convective regime).

Note that for cases 1 and 3 the 'plastic viscosity' does not contribute to the viscosity at all and one should set $\mu = \mu_{lin}$.

4 Two-dimensional convection in a unit box

This benchmark deals with the 2-D thermal convection of a fluid of infinite Prandtl number in a rectangular closed cell, identical to the first computer practical.

The temperature is fixed to zero on top and to ΔT at the bottom, with reflecting symmetry at the sidewalls (i.e. $\partial_x T = 0$) and there are no internal heat sources. Free-slip conditions are implemented on all boundaries.

The Rayleigh number is given by

$$Ra = \frac{\alpha g_y \Delta T h^3}{\kappa\nu} = \frac{\alpha g_y \Delta T h^3 \rho^2 c_p}{k\mu} \tag{16}$$

In what follows, I use the following parameter values: $L_x = L_y = 1$,$\rho_0 = c_P = k = \mu = 1$, $T_0 = 0$, $\alpha = 10^{-4}$, $g = 10^4 Ra$.

The initial temperature field is given by

$$T(x,y) = (1-y) + 0.01\cos(\pi x/L_x)\sin(\pi z/L_z) \tag{17}$$

The perturbation in the initial temperature fields leads to a perturbation of the density field and sets the fluid in motion. Depending on the initial Rayleigh number, the system ultimately reaches a steady state after some time.

The root mean square of the velocity field in the whole domain is defined as follows:

$$v_{rms} = \left(\frac{1}{V_\Omega} \int_\Omega |\boldsymbol{v}|^2 \, dV \right)^{1/2} \tag{18}$$

The Nusselt number (i.e. the mean surface temperature gradient over mean bottom temperature) is computed as follows [2]:

$$Nu = L_y \frac{\int \frac{\partial T}{\partial y}(y = L_y) dx}{\int T(y=0) dx} \tag{19}$$

Note that in our case the denominator is equal to 1 since $L_x = 1$ and the temperature at the bottom is prescribed to be 1.

We will consider five cases, presented in the table 2

5 How to

The code is to be downloaded there `http://cedricthieulot.net/mantledynamics.html` .

Move the `.tar` file to the location of your choice. Then untar the file as follows:

```
> tar -xvf code_lab2.tar
```

In order to compile the code, you only have to type

```
> make
```

In order to run the code, you only have to type

```
> ./simplefem
```

Please open `simplefem.f90` with the text editor of your choice and look carefully at the code. Determine where the inputs are given, how and where the outputs are written. Also have a look at the `viscosity.f90` which you will have to modify.

Note that in between each run you can (should ?) erase all previously obtained data with

```
> ./clean
```

6 Experiments

- compute $\sqrt{\dot{\epsilon} : \dot{\epsilon}}$ in the viscosity subroutine.
- look at the 'geval' parameter in simplefem.f90, where it is given a value, and where it is used. It should correspond to the cases 1,2,3,4,5 of Table 2. Declare and assign values to several parameters in the *viscosity* function corresponding to γ_T, γ_z, and $\mu^\star$. Use a *select case* fortran command to implement the various rheologies required for the 5 cases to be run.
- Make sure that computed viscosities cannot fall outside of the range $[10^{-5} - 2]$.
- For cases 1,2,3,4 produce paraview plots of the temperature, viscosity ($\log_{10}$) and velocity at steady state. Plot the root mean square velocity and the Nusselt number as a function of time. Discuss all graphs per case, and compare them across all four cases. Case 1 takes quite some time to reach steady state, the others are much quicker. Also plot the average temperature profiles.
- For case 5, vary σ_y from 3 to 6. Somewehere in this range you should obtain a periodic system. What are the values of σ_y corresponding to mobile lead to periodic, and to periodic to stagnant lid ? Plot the vrms and Nu as a function of time in the case of an episodic experiment. What is the period ? On a graph with σ_y as x coordinate and Nu as y coordinate, report the single Nu value for steady state experiments, and the min/max Nu for the episodic experiments. Such a plot is called a bifurcation diagram.
- if you have time left or if you are curious enough: Look at the influence of resolution on all the results, and especially on the bifurcation experiment. For case 5, and in the case of an epsiodic/periodic experiment, plot the the Nusselt number as a function of the vrms. What do we observe ?

References

[1] K.-J. Bathe. *Finite Element Procedures in Engineering Analysis.* Prentice-Hall, 1982.

[2] B. Blankenbach, F. Busse, U. Christensen, L. Cserepes, D. Gunkel, U. Hansen, H. Harder, G. Jarvis, M. Koch, G. Marquart, D. Moore, P. Olson, H. Schmeling, and T. Schnaubelt. A benchmark comparison for mantle convection codes. *Geophys. J. Int.*, 98:23–38, 1989.

[3] C. Cuvelier, A. Segal, and A.A. van Steenhoven. *Finite Element Methods and Navier-Stokes Equations.* D. Reidel Publishing Company, 1986.

[4] D.R. Davies, C.R. Wilson, and S.C. Kramer. Fluidity: A fully unstructured anisotropic adaptive mesh computational modeling framework for geodynamics. *Geochem. Geophys. Geosyst.*, 12(6), 2011.

[5] Jean Donea and Antonio Huerta. *Finite Element Methods for Flow Problems.* John Wiley & Sons, 2003.

[6] T.V. Gerya and D.A. Yuen. Characteristics-based marker-in-cell method with conservative finite-differences schemes for modeling geological flows with strongly variable transport properties. *Phys. Earth. Planet. Inter.*, 140:293–318, 2003.

[7] M. Gunzburger. *Finite Element Methods for Viscous Incompressible Flows: A Guide to Theory, Practice and Algorithms.* Academic, Boston, 1989.

[8] T.J.R. Hughes. *The Finite Element Method. Linear Static and Dynamic Finite Element Analysis.* Dover Publications, Inc., 2000.

[9] S. King, C. Lee, P. van Keken, W. Leng, S. Zhong, E. Tan, N. Tosi, and M. Kameyama. A community benchmark for 2D Cartesian com- pressible convection in the Earths mantle. *Geophy. J. Int.*, 180:7387, 2010.

[10] M. Kronbichler, T. Heister, and W. Bangerth. High accuracy mantle convection simulation through modern numerical methods . *Geophy. J. Int.*, 191:12–29, 2012.

[11] W. Leng and S. Zhong. Implementation and application of adaptive mesh refinement for thermochemical mantle convection studies. *Geochem. Geophys. Geosyst.*, 12(4), 2011.

[12] R.W. Lewis, P. Nithiarasu, and K.N. Seetharamu. *Fundamentals of the Finite Element Method for Heat and Fluid Flow.* John Wiley & Sons, Ltd, 2004.

[13] C. Stein, J. Lowman, and U. Hansen. A comparison of mantle convection models featuring plates. *Geochem. Geophys. Geosyst.*, 15:2689–2698, 2014.

[14] R.A. Trompert and U. Hansen. Mantle convection simulations with rheologies that generate plate-like behaviour . *Nature*, 395:686–689, 1998.

[15] O.C. Zienkiewicz and R.L. Taylor. *The Finite Element Method. Vol. 1,2,3.* Butterworth and Heinemann, 2002.