MEEUUW
Mantle modelling Early Earth Utrecht University Work in progress

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1 Foreword

I have quite a history of naming codes and regretting it afterwards. This is one more in my collection: SoPHa, SPHene, FANTOM, ELEFANT, FLAPS, FieldStone.

2 Install process

The code consists of a dozen of Python files. Aside from standard Python modules (numpy, scipy, etc ...) the numba[1] package is needed and needs to be installed. The reason for the use of this module is as follows: "Numba translates Python functions to optimized machine code at runtime using the industry-standard LLVM compiler library. Numba-compiled numerical algorithms in Python can approach the speeds of C or FORTRAN. You don't need to replace the Python interpreter, run a separate compilation step, or even have a C/C++ compiler installed. Just apply one of the Numba decorators to your Python function, and Numba does the rest." [Taken from the numba website]

If numba is not available on your machine, simply delete all occurences of `@numba.njit` before the functions.

3 Philosophy

The code is entirely written in Python. The domain is only 2d, although an axisymmetric option has been implemented. The code is not meant to compete with ASPECT or any similar code. It is meant to be an educational tool, typically for MSc or PhD students in mind. The interface is simple and flexible. Inside a experimentX.py file the user needs to specify the necessary parameters (e.g. the resolution, domain size, number of timesteps, etc ...) and fill in a few template functions:

```
initial_temperature
assign_boundary_conditions_V
assign_boundary_conditions_T
particle_layout
material_model
gravity_model
```

There are at the moment 10 so-called experiments (called cookbooks in ASPECT) that either aim at reproducing existing articles results (numerical benchmarks) or built as setups to be used in class. Each experiment is entirely contained in its corresponding experimentX.py file. The current list of experiments is as follows:

```
# experiment  0: Blankenbach et al, 1993 - isoviscous convection
# experiment  1: van Keken et al, JGR, 1997 - Rayleigh-Taylor experiment
# experiment  2: Schmeling et al, PEPI 2008 - Newtonian subduction
# experiment  3: Tosi et al, 2015 - visco-plastic convection
# experiment  4: not sure. mantle size convection
# experiment  5: Trompert & Hansen, Nature 1998 - convection w/ plate-like
# experiment  6: Crameri et al, GJI 2012 (cosine perturbation & plume)
# experiment  7: ESA workshop
# experiment  8: quarter - sinker
# experiment  9: axisymmetric Mars setup
# experiment 10: axisymmetric aspect benchmark of Stokes sphere
```

[1] https://numba.pydata.org/

The results obtained with the code for these experiments are available in the `RESULTS` folder.

In order to select one of these experiments, simply open meeuuw.py and edit line 55 which reads experiment=X.

In order to run the code, simply then type the following in the terminal:

```
python3 meeuuw.py
```

Note that a script carrying this also exists and can be executed as follows:

```
./run
```

The code will then run and will produce *a lot* of information while running in the terminal. If you wish to keep this information you can redirect the screen output to a file as follows for example:

```
python3 meeuuw.py > screen_output.text
```

The code also generates `.ascii` files (to be plotted with gnuplot for example) and `.vtu` files to be opened with ParaView. All are placed automatically in the `OUTPUT` folder.

After a simulation, if results are to be discarded, and before running a new model, it is recommended to remove all results by running the following script:

```
./cleandata
```

4 Numerical methods

The Stokes equations are discretised by means of the Finite Element Method (FEM). As explained in Thieulot et al. (2022) and Thieulot et al. (2022), there are many so-called element pairs for the velocity and pressure spaces, and we here rely on quadrilateral Taylor-Hood elements only, i.e. $Q_2 \times Q_1$. The energy equation relies on Q_2 elements for the temperature.

The FEM formulation of these equations is explained in the FieldStone manual[2].

[2] `https://cedrict.github.io/`

5 Code structure

```
- quadrature rule points and weights
- open output files & write headers
- build velocity nodes coordinates
- connectivity for velocity nodes
- build pressure grid
- build pressure connectivity array
- define velocity boundary conditions
- define temperature boundary conditions
- initial temperature. T is a vector of float64 of size nn_V
- compute area of elements / sanity check
- precompute basis functions values at quadrature points
- precompute basis functions values at V nodes
- compute coordinates of quadrature points - xq,yq are size (nel,nqel)
- compute gravity vector at quadrature points -  gxq,gyq are size (nel,nqel)
- compute gravity on mesh points
- compute normal vector of domain
- compute array for assembly
- fill II_V,JJ_V arrays for Stokes matrix
- fill II_T,JJ_T arrays for temperature matrix & plith matrix
- particle coordinates setup
- particle paint
- particle layout
- --------------------- time stepping loop ---------------------------------
    - interpolate strain rate on particles
    - interpolate temperature on particles
    - evaluate density and viscosity on particles (and hcond, hcapa, hprod)
    - project particle properties on elements
    - project particle properties on V nodes
    - remove nodal rho profile
    - project nodal values onto quadrature points
    - split solution into separate u,v,p velocity arrays
    - convert velocity to polar coordinates
    - compute timestep
    - normalise pressure: simple approach to have avrg p = 0 (volume or surface)
    - project Q1 pressure onto Q2 (vel,T) mesh
    - project velocity on quadrature points
    - build temperature matrix
    - solve temperature system
    - compute vrms
    - compute nodal heat flux
    - compute heat flux and Nusselt at top and bottom
    - compute temperature profile
    - compute nodal strainrate
    - compute nodal deviatoric strainrate
    - compute stress tensor components
    - compute dynamic topography at bottom and surface topo
    - compute nodal pressure gradient
    - advect particles
    - locate particles and compute reduced coordinates
    - compute strain on particles
    - export min/max coordinates of each material in one single file
    - generate/write in pvd files
    - export solution to vtu file
    - export particles to vtu file
    - export quadrature points to vtu file
    - compute gravitational field above domain
    - assess steady state
- --------------------- end time stepping loop -----------------------------
```

6 Generic mass, momentum, energy conservation equations

We focus on the system of equations in a $d = 2$- or $d = 3$-dimensional domain Ω that describes the motion of a highly viscous fluid (i.e. near infinite Prandlt number) driven by differences in the gravitational force due to a density variations. In the following, we largely follow the exposition of this material in Schubert, Turcotte and Olson Schubert et al. 2001.

Specifically, we consider the following set of equations for velocity $\vec{\mathrm{v}}$, pressure p and temperature T:

$$-\vec{\nabla}p + \vec{\nabla}\cdot\left[2\eta\left(\dot{\varepsilon}(\vec{\mathrm{v}}) - \frac{1}{3}(\vec{\nabla}\cdot\vec{\mathrm{v}})\mathbf{1}\right)\right] + \rho\vec{g} = \vec{0} \qquad \text{in } \Omega, \quad (1)$$

$$\frac{\partial\rho}{\partial t} + \vec{\nabla}\cdot(\rho\vec{\mathrm{v}}) = 0 \qquad \text{in } \Omega, \quad (2)$$

$$\rho C_p\left(\frac{\partial T}{\partial t} + \vec{\mathrm{v}}\cdot\vec{\nabla}T\right) - \vec{\nabla}\cdot k\vec{\nabla}T = \rho H + 2\eta\left(\dot{\varepsilon}(\vec{\mathrm{v}}) - \frac{1}{3}(\vec{\nabla}\cdot\vec{\mathrm{v}})\mathbf{1}\right) : \left(\dot{\varepsilon}(\vec{\mathrm{v}}) - \frac{1}{3}(\vec{\nabla}\cdot\vec{\mathrm{v}})\mathbf{1}\right) \quad (3)$$

$$+ \alpha T\left(\frac{\partial p}{\partial t} + \vec{\mathrm{v}}\cdot\vec{\nabla}p\right) \qquad \text{in } \Omega, \quad (4)$$

where $\dot{\boldsymbol{\varepsilon}}(\vec{\mathrm{v}}) = \frac{1}{2}(\vec{\nabla}\vec{\mathrm{v}} + \vec{\nabla}\vec{\mathrm{v}}^T)$ is the symmetric gradient of the velocity (often called the *strain rate* tensor).

In this set of equations, (1) and (2) represent the compressible Stokes equations in which $\vec{\mathrm{v}} = \vec{\mathrm{v}}(\mathbf{x}, t)$ is the velocity field and $p = p(\mathbf{x}, t)$ the pressure field. Both fields depend on space $\mathbf{x}$ and time t. Fluid flow is driven by the gravity force that acts on the fluid and that is proportional to both the density of the fluid and the strength of the gravitational pull.

Coupled to this Stokes system is equation (3) for the temperature field $T = T(\mathbf{x}, t)$ that contains heat conduction terms as well as advection with the flow velocity $\vec{\mathrm{v}}$. The right hand side terms of this equation correspond to

- internal heat production for example due to radioactive decay;
- friction (shear) heating;
- adiabatic compression of material;

7 Equation of state

The equation of state gives the density as a function of the pressure and temperature: $\rho = \rho(p, T)$. The density is then either obtained from precomputed lookup tables or a simpler functional approach is often taken by means of a linearisation.

The widely used Boussinesq approximation (see below) linearizes these basic conservation laws near the reference hydrostatic state. If density changes caused by the pressure deviations $p' = p - p_0$ are neglected, we may linearize the state equation with respect to the temperature deviations $T - T_0$, where T_0 is a reference temperature, and write:

$$\rho = \rho_0(1 - \alpha(T - T_0))$$

This approximation thus means that the influence of hydrostatic pressure (as well as temperature T_0) on density is hidden in 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, that is, neglecting thermal expansion, we arrive at the simplified equation:

$$\vec{\nabla} \cdot (\rho_0 \vec{\mathrm{v}}) = 0$$

8 Anelastic liquid approximation (ALA)

This comes from Matyska et al. (2007).

If we assume that there is a reference hydrostatic state characterized by $\vec{\mathrm{v}} = 0$ in which the hydrostatic pressure p_0, hydrostatic density ρ_0, and hydrostatic gravity acceleration g_0 are related by $\vec{\nabla} p_0 = \rho_0 \vec{g}_0$, and moreover that pressure deviations $p' = p - p_0$ are negligible in the heat equation, the transfer of heat in a homogeneous material (i.e., entropy may be considered as a function of only p and T) is then described by the well-known equation:

$$\rho C_p \left(\frac{\partial T}{\partial t} + \vec{\mathrm{v}} \cdot \vec{\nabla} T \right) = \vec{\nabla} \cdot k \vec{\nabla} T - \alpha T \vec{\mathrm{v}} \cdot \rho \vec{g} + \boldsymbol{\tau} : \vec{\nabla} \vec{\mathrm{v}} + Q$$

where C_p is the isobaric specific heat, α is the thermal expansion coefficient and vr denotes the radial component of velocity. The left-hand side of equation 8 represents local changes of heat balance; the second (third) term on the right-hand side describes ad- vection of heat (adiabatic heating and/or cooling).

9 Boussinesq approximation (BA)

In the case of an incompressible flow, then $\partial\rho/\partial t = 0$ and $\vec{\nabla}\rho = 0$, i.e. $D\rho/Dt = 0$ and the mass conservation equation becomes:

$$\vec{\nabla} \cdot \vec{\mathbf{v}} = 0$$

A vector field that is divergence-free is also called solenoidal[3].

In this case the equations above can now be written

$$-\vec{\nabla}p + \vec{\nabla} \cdot [2\eta\left(\dot{\boldsymbol{\varepsilon}}(\vec{\mathbf{v}})\right)] + \rho\vec{g} = \vec{0} \qquad \text{in } \Omega, \tag{5}$$

$$\vec{\nabla} \cdot \vec{\mathbf{v}} = 0 \qquad \text{in } \Omega, \tag{6}$$

$$\rho C_p \left(\frac{\partial T}{\partial t} + \vec{\mathbf{v}} \cdot \vec{\nabla}T\right) - \vec{\nabla} \cdot k\vec{\nabla}T = \rho H + 2\eta\dot{\varepsilon}(\vec{\mathbf{v}}) : \dot{\varepsilon}(\vec{\mathbf{v}}) + \alpha T \left(\frac{\partial p}{\partial t} + \vec{\mathbf{v}} \cdot \vec{\nabla}p\right) \qquad \text{in } \Omega, \tag{7}$$

As nicely explained in Spiegel et al. (1960):

> In the study of problems of thermal convection it is a frequent practice to simplify the basic equations by introducing certain approximations which are attributed to Boussinesq (1903). The Boussinesq approximations can best be summarized by two statements:
>
> 1. The fluctuations in density which appear with the advent of motion result principally from thermal (as opposed to pressure) effects.
> 2. In the equations for the rate of change of momentum and mass, density variations may be neglected except when they are coupled to the gravitational acceleration in the buoyancy force."

Note that their paper examines the Boussinesq approximation for compressible fluids.

The Boussinesq approximation assumes that the density can be considered constant in all occurrences in the equations with the exception of the buoyancy term on the right hand side of (1). The primary result of this assumption is that the continuity equation (2) will now read $\vec{\nabla} \cdot \vec{\mathbf{v}} = 0$. This implies that the strain rate tensor is deviatoric. Under the Boussinesq approximation, the equations are much simplified:

$$-\vec{\nabla}p + \vec{\nabla} \cdot [2\eta\dot{\boldsymbol{\varepsilon}}(\vec{\mathbf{v}})] + \rho\vec{g} = \vec{0} \qquad \text{in } \Omega, \tag{8}$$

$$\vec{\nabla} \cdot \vec{\mathbf{v}} = 0 \qquad \text{in } \Omega, \tag{9}$$

$$\rho_0 C_p \left(\frac{\partial T}{\partial t} + \vec{\mathbf{v}} \cdot \vec{\nabla}T\right) - \vec{\nabla} \cdot k\vec{\nabla}T = \rho H \qquad \text{in } \Omega \tag{10}$$

Note that all terms on the rhs of the temperature equations have disappeared, with the exception of the source term.

In Zelst et al. (2022) we read:

> The Boussinesq approximation (Oberbeck (1879); Boussinesq, 1903; Rayleigh, 1916) assumes that density variations are so small that they can be neglected everywhere except in the buoyancy term in the momentum equation, which is equivalent to using a constant reference density profile. This implies incompressibility [...]. In addition, adiabatic heating and shear heating are not considered in the energy equation. This approximation is valid as long as density variations are small and the modelled processes would cause no substantial shear or adiabatic heating. The Boussinesq approximation is often used in lithosphere-scale models. Due to its simplicity, the approximation of in- compressibility is sometimes also adopted for whole-mantle convection models, wherein it is only approximately valid, and it has been shown that compressibility can have a large effect on the pattern of convective flow Tackley 1996.

[3] https://en.wikipedia.org/wiki/Solenoidal_vector_field

10 Extended Boussinesq approximation (EBA)

In Zelst et al. (2022) we read:

> The extended Boussinesq approximation (Christensen et al. 1985; Oxburgh et al. 1978) is based on the same assumptions as the BA but does consider adiabatic and shear heating. Since it includes adiabatic heating, but not the associated volume and density changes, it can lead to artificial changes of energy in the model, i.e. material is being heated or cooled based on the assumption that it is compressed or it expands, but the mechanical work that causes compression or expansion is not done. Consequently, the extended Boussinesq approximation should only be used in models without substantial adiabatic temperature changes.
>
> For a comparison between some of these approximations using benchmark models, see e.g. Steinbach et al. (1989), Leng et al. (2008), King et al. (2010), Gassmöller et al. (2020). In addition, the choice of approximation may also be limited by the numerical methods being employed (for example, the accuracy of the solution for the variables that affect the density). Also note that, technically, these approximations are all internally inconsistent to varying degrees, since they do not fulfil the definitions of thermodynamic variables but use linearised versions instead, and they use different density formulations in the different equations. Nevertheless, many of them are generally accepted and widely used in geodynamic modelling studies, as they allow for simpler equations and more easily obtained solutions.

11 Initial adiabatic temperature profile

12 Dynamic topography

References

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