

Viscous modelling of the upper mantle

Timothy Gray 2 November 2021

Why numerical modelling?

Because we have no other choice!

Numerical modelling is the **only** way to investigate the evolution of the mantle and lithosphere when no data is available.



Deepest borehole ever drilled - 12km



Seismic data can penetrate deeper but cannot provide insight into Earth's evolution

Numerical modelling uses **fundamental** physical laws to investigate the Earth's evolution over different spatial and temporal scales

Governing equations

The governing equations for modelling of the upper mantle must fundamentally follow conservation of mass and momentum.

By considering a small packet of material, we can derive an equation describing conservation of mass.

Continuity equation (Eulerian form):

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

In words:

Mass out – mass in = change of mass in the packet

Continuity equation (incompressible):

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

Introduction to Numerical Geodynamic Modelling, Gerya, 2018



Governing equations

Likewise, momentum must be conserved across our packet of material. This is in effect a statement of Newton's second law, F=ma.

Momentum equation (Eulerian form):

$$\frac{\partial \sigma_{ij}}{\partial x_j} + \rho g_i = \rho \left(\frac{\partial v_i}{\partial t} + v_i \frac{\partial v_i}{\partial x_j} \right)$$

In words:

Stress on the body + the force of gravity

= the acceleration of the body



Constitutive law

From the fundamental equations of continuity and conservation of momentum, there are several directions we can go in.

These directions depend on the constitutive law, which relates stress to strain.

The simplest is Newton's law of viscosity.

Newton's law of viscosity:

$$\tau = \eta \frac{\partial v}{\partial x}$$

In words:

Shear stress is linearly proportional to shear strain rate.



Newtonian viscosity

Newton's law of viscosity:

$$\tau = \eta \frac{\partial v}{\partial x}$$



Why is it valid?

On very long timescales (1000's of years and more), solid rock can act as a fluid due to creep.

Typical viscosites of the upper mantle range from 1e20 Pa.s to 1e25 Pa.s in the crust.

Why isn't it valid?

Because rocks do still behave as elastic solids on short time scales – we know this because S waves exist. Viscous rocks are a good assumption, but an assumption nonetheless.

More on this later.

Applying Newtonian viscosity

Before, we had the general stress tensor. Let's first split it into normal and deviatoric components.

$$\sigma_{ij}' = \sigma_{ij} + P\delta_{ij}$$

Where we introduce the pressure, P. Similarly for the strain rate tensor: $\hat{\epsilon}_{i}$

$$_{ij} = \frac{1}{2} \left(\frac{\partial y_i}{\partial x_j} + \frac{\partial y_j}{\partial x_i} \right)$$

$$\dot{\epsilon}_{ij}' = \dot{\epsilon}_{ij} + \delta_{ij} \frac{1}{3} \dot{\epsilon}_{kk}$$

Under this formulation, the Newtonian viscosity constitutive law can be written as:

$$\sigma_{ij}' = 2\eta \dot{\epsilon}_{ij}'$$

The Navier Stokes equations

The result of our work is the derivation of the Navier Stokes equations in 3D for an incompressible, viscous fluid.

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = \eta \nabla^2 \mathbf{v} - \nabla P + \rho \mathbf{g}$$
$$\nabla \cdot \mathbf{v} = 0$$

This equation forms the basis for most fluid dynamics on everyday scales, where compressibility is negligible and Newtonian viscosity is assumed.

Solving the Navier Stokes equations

Unfortunately, the Navier Stokes equations are difficult to solve analytically - \$1 million prize if you do! Numerical solutions are required. Gateway to the world of CFD – computational fluid dynamics

Many methods available:

- Finite differences
- Finite element method
- Smoothed particle hydrodynamics
- Spectral methods



The Stokes equations

Typically, we work with fluids that that are moving *very* slowly. In this case, we can eliminate the inertial terms on the left hand side completely, giving us the Stokes equations for creeping viscous flow:

$$\eta \nabla^2 \mathbf{v} = \nabla P + \rho \mathbf{g}$$
$$\nabla \cdot \mathbf{v} = 0$$

The Stokes equations are linear, and much easier to solve. Analytical solutions exist for simple cases. However, it's still not trivial and numerical solutions are still usually required.

The Heat Equation

We can introduce temperature in our model using the well known **heat equation**, which is based on conservation of heat energy:

$$\rho C_P \left(\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) - k \nabla^2 T = H_s$$

In words:

The change in heat of the body is the result of **internal heating**, **diffusion**, and **advection**.

Internal heating can arise from **radiogenic heating**, **shear heating**, **adiabatic heating**, or heat arising from **phase changes**.

Diffusion depends on thermal conductivity of the material.

Advection is heat transport by bulk motion of material.

Domain, initial, and boundary conditions

Before modelling can begin, you should carefully consider your modelling **domain**. This is determined by your research question.

Boundary conditions may include free slip, stress free, or even free surface conditions.

Initial conditions are also important and influenced by your research question.



2D or 3D?

Cartesian or spherical?

Initial temperature?

Is the Earth actually flat?



The first numerical models

Early models of mantle convection date to the late 1960s.

"Convection in a Variable Viscosity Fluid Heated from Within", Foster, 1969

- Considers 2D two-layered Newtonian viscous convection with viscosity contrast, internal heating.





Fig. 6. Time development of the horizontally averaged temperature profile for an initially hot fluid (1000°C), $\Re = 10^8$, and $\gamma = 15$ at preferred horizontal wave number.

Spectral methods

Early studies did not have access to fast computers that we have today.

One possible workaround is to use spectral methods. Instead of representing a solution directly, it is possible to represent it as a series:

$$f(x) = \sum_{n=0}^{N} F_n \exp(i2\pi nx/L)$$

Instead of manipulating f(x) directly, it may be easier to manipulate the series coefficients. The series can be truncated if faster computational time is desired.

Alternative bases such as the spherical harmonics, or Chebychev polynomials may be used.

Who would win?



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Tackley et al., 1993 – Spectral methods in 3D



FIG. 1 Cold downwellings for final frame of simulation. Blue surface is an isocontour showing where the temperature is 110 K lower than the horizontally averaged value. Green surface is the core. A network of interconnected linear downwellings is visible in the upper mantle, with three huge cylindrical downwellings in the lower mantle, spreading out into pools of cold material above the core-mantle boundary.



FIG. 2 Hot upwellings for final frame of simulation. Red surface is an isocontour of superadiabatic temperature, showing where the temperature is 110 K higher than the reference-state adiabat. A single plume from the core-mantle boundary feeds a hot region in the upper mantle. Note that most broad hot regions in the upper mantle are not directly linked to lower-mantle structures.

Downsides of spectral methods

Spectral methods suffer from downsides which have made their use rare in recent years.

- Gibbs phenomenon overshoot
- Laterally varying viscosity contrasts difficult to implement
- Less logical to implement for less mathematically inclined people
- Performance gains negated by increase in computational power
- Still used in certain applications (e.g. magnetohydrodynamic core modelling)



Finite differences

One of the simplest ways is to use finite differences. Derivatives are discretised – we can visualise this in 2D with the use of a grid.

Discretisation:

$$\frac{dy}{dx} \approx \frac{y_1 - y_{-1}}{\Delta x} \quad \frac{d^2y}{dx^2} \approx \frac{y_1 - 2y_0 + y_{-1}}{\Delta x^2}$$

Sometimes things to not 'line up' perfectly – a staggered grid minimises errors.

The result of discretisation is a linear system of equations, which can be solved using one of many existing solvers.

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2D implementation of visco-elasto-plastic rheology



Fig. 13.2 Staggered 2D irregularly spaced numerical grid corresponding to the algorithm presented in Fig. 13.1.

Finite element method

The relatively simple finite difference is extended to complex geometries by the **finite element method**.

The region is divided into elements, and basis functions are chosen to represent the solution in each element. The result is again a system of linear equations.









Modern methods - I3ELVIS

Plate tectonics on the Earth triggered by plumeinduced subduction initiation, Gerya et al., Nature, 2015





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Modern methods - StagYY

StagYY is a global scale code which can be run in 3D using a tennis-ball like Yin-Yang grid.

A free plate surface and weak oceanic crust produce single-sided subduction on Earth, Crameri et al. 2012





Determining viscosity

The viscosity of rocks depends on temperature, pressure, grain size, and stress.

Physically, rocks deform through creep mechanisms:

Diffusion creep – diffusion of atoms through the mineral lattice, either through the crystal or at grain boundaries. Temperature, but not stress dependent.

Dislocation creep – migration of dislocations (imperfections in lattice structure). More stress dependent.





Determining viscosity

The viscosity of rocks depends on temperature, pressure, grain size, and stress.

A simple model with temperature and pressure dependence is the Arrhenius model:

$$\eta(T,P) = \eta_0 \exp\left(\frac{E_a + PV_a}{RT}\right)$$

More complex models exist, such as the following incorporating grain size and stress (second stress tensor invariant) dependence (Gerya, 2019):

$$\eta_{eff} = F_1 \frac{1}{A_D h^m (\sigma_{II})^{(n-1)}} \exp\left(\frac{E_a + V_a P}{RT}\right)$$

Further models based on empirical results are also available.

Limitations of viscous rheology

Viscous rheology is limited.

- Rocks behave elastically on short time scales
- Fast processes cannot be captured by viscous rheology.
- Cold rocks (such as in the lithosphere) exhibit brittle or plastic deformation rather than viscous deformation.
- Ideally, a visco-elasto-plastic rheology would be used that can capture the 'true' rheology of rocks at different time scales.



Fig. 12.2. Reversible deformation of initially unstressed (a) elastic slab surrounded by a weak viscous medium (Gerya and Yuen, 2007). Deformation of the slab in (b) is caused by a vertical gravity field. When gravity is 'removed', the deformed slab recovers its original shape (c) while the surrounding medium remains deformed since viscous deformation is irreversible.

Alternative rheological models

Earlier we implemented Newtonian viscosity into our model. Let's consider some alternatives:

Viscous rheology - stress is proportional to strain rate

$$\sigma'_{ij} = 2\eta \dot{\epsilon}'_{ij}$$

Elastic rheology - stress is proportional to strain

General:
$$\sigma_{ij} = C_{ijkl} \epsilon_{kl}$$
 isotropic: $\sigma_{ij} = \lambda \delta_{ij} \epsilon_{kk} + 2\mu \epsilon_{ij}$

Maxwell rheology – simplest viscoelastic rheology combining instantaneous deformation and viscous deformation.

Visco-elasto-plastic rheology - Incorporates plasticity into viscoelastic models – stresses greater than yield stress will cause plastic deformation of the material.

$$\dot{\epsilon}_{II} = A_{Peierls} \sigma_{II}^2 \exp\left\{-\frac{E_a + PV_a}{RT} \left[1 - \left(\frac{\sigma_{II}}{\sigma_{Peierls}}\right)^k\right]^q\right\}$$





- Numerical modelling is a **necessary tool** for understanding the Earth's interior.
- Conservation of mass, momentum, and heat form the fundamental basis for the equations we use.
- Choice of a suitable rheology dictates the equations we end up with linear (Newtonian) viscosity is a suitable choice for many applications in the Earth's mantle.
- Many methods exist for solving the fundamental equations.
- Limitations to the viscous approximation mean that in certain circumstances it is necessary to use more complex rheologies.