# Introduction

**Theory:** What is this book? What this book is not. Get started. Seven golden rules to learn the topic. Short history of geodynamics and numerical geodynamic modelling. Few words about programming and visualisation. Nine programming rules.
**Exercises:** Starting with MATLAB. Visualisation exercise.

## What is this book?

This book is a practical, hands-on introduction to numerical geodynamic modelling for inexperienced people, i.e. for young students and newcomers from other fields. It does not require much background in mathematics or physics and is therefore written with a maximum amount of simple technical details. If you are inexperienced – this book is for you!

## What this book is not

This book is not a treatise or a compendium of knowledge for experienced researchers. It does not contain large overviews of existing numerical techniques and only simple approaches are explained. If you are experienced in numerical methods, read Chapter 17 first and then decide if you wish to read about the technical details presented in previous chapters.

## Get started

Already decided?! Then let us get started! In recent decades numerical modelling has become an essential approach in geosciences in general and in geodynamics in particular. This is a very natural process ('instinctive evolution') since direct human observation scales are extremely limited in both time and space (depth) and rapid progress in computer technology offers every day new and exceptional possibilities to explore sophisticated mathematical models and this is true in every discipline, and even industrial applications. Numerical modelling in geosciences is widely used for both testing and generating hypotheses and strongly pushing geology from an observational, intuitive to a deductive, predictive natural science. Geo-modelling and geo-visualisation play a strong role in relating different branches of geosciences. Therefore, it has become necessary to have some knowledge about numerical techniques before planning and conducting state-of-the-art interdisciplinary research in any branch of geosciences. In this respect, geodynamics is traditionally 'infected' by numerical modelling and promotes the progress of numerical methods in geosciences.

Before starting with numerical modelling we should consider one of the very popular 'myths' among geologists, who often declare (or think) something like:

*Numerical modelling is very complicated; it is too difficult for people with a traditional geological background and should be performed by mathematicians.*

I used to think like that before I started. I always remember my feeling when I heard for the first time the expression, 'Navier–Stokes equation'. 'Ok, forget it! This is hopeless,' I thought at that time, and that was wrong. Therefore, let me formulate the seven 'golden rules' elaborated during my learning experience.

**Golden Rule 1.** ***Numerical modelling is simple and is based on simple mathematics.***

All you need to know is:

- linear algebra,
- derivatives.

Most of the 'complicated' mathematical knowledge is learned in school before we even start to study at university! I often say to my students that all is needed is:

strong MOTIVATION,
usual MATHS,
clear EXPLANATIONS,
regular EXERCISES.
Motivation is most important, indeed . . .

**Golden Rule 2.** ***When numerical modelling looks complicated see Rule 1.***

**Golden Rule 3.** ***Numerical modelling consists of solving partial differential equations (PDEs).***

There are only a few equations to learn (e.g. Lynch, 2005). They are generally not complicated, but it is essential to learn and understand them gradually and properly.

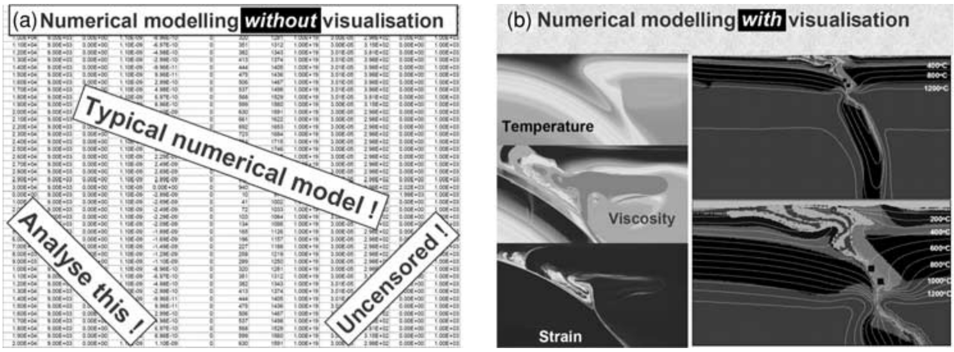


Fig. Introduction.1 Rule 6: Visualisation is important!

For example, to model the broad spectrum of geodynamic processes discussed in this book, it is necessary to know three principal conservation PDEs only:

- the equation of continuity (conservation of mass),
- the equation of motion (conservation of momentum – *Navier–Stokes equation!*)
- the temperature equation (conservation of heat).

So, only *three* equations have to be understood and not tens or hundreds of them!

**Golden Rule 4.** ***Read books on numerical methods several times.***

There are many excellent books on numerical methods. Most of these books are, however, written for physicists and engineers and need effort to be 'digested' by people with a traditional geological background.

**Golden Rule 5.** ***Repeat transformations of equations involved in numerical modelling.***

These transformations are generally standard and trivial, but repeating them develops a familiarity with the PDEs (maybe you will even start to like them . . . ), and allows you to understand the structure of the different PDEs. This book, by the way, is full of such trivial detailed transformations – follow them too.

**Golden Rule 6.** ***Visualisation is important!***

Without proper visualisation of results, almost nothing can be done with numerical modelling (Fig. Introduction.1). Modellers often spend more time on visualisation than on computing and programming.

**Golden Rule 7**. ***Ask!***

This is the most efficient way of learning. In numerical geodynamic modelling also many small hints and details exist. They are extremely important, but rarely discussed in publications (in contrast to this book).

### Short history of geodynamics and numerical geodynamic modelling

The numerical modelling approaches discussed in this book are adopted for solving *thermomechanical* geodynamic problems. Geodynamics – dynamics of the Earth – is a core geological subject that was very actively progressing during the last century, especially since the establishment of plate tectonics in the 1960s. This was a really great time for geology that 'drifted' strongly from a descriptive (qualitative) field, to a predictive (quantitative) physical science. The overall history of the development of geodynamics was not, indeed, very 'dynamic' but rather slow and complicated. A brilliant introduction to this field (which I strongly recommend you to read) is written by Donald L. Turcotte and Gerald Schubert (2002). According to this introduction and other sources, the following steps were historic in understanding the Earth as a dynamic system:

**1620:** *Francis Bacon pointed out the similarity in shape between the west coast of Africa and the east coast of South America.*

This was about 400 years ago (!) and several centuries were needed to start interpreting this similarity.

**1665:** *Athanasius Kircher, in his two-volume* 'Mundus subterraneus'*, probably the first printed work on geophysics and vulcanology, held that much of the phenomena on earth were due to the fact that there is 'fire' under the terra firma.*

This was, indeed, very unusual teaching for those days (about 350 years ago!) and very much in line with the thermal origin of the mantle convection.

**Early part of eighteenth century:** *Gottfried Wilhelm Leibniz proposed that the Earth has a molten core and anticipated the igneous nature of the mantle.*

The understanding of the Earth as a hot layered planetary body. One should really have a vision to guess this around 300 years ago!

**Latter part of the nineteenth century:** *Establishing the fluid-like behaviour of the Earth's mantle based on gravity studies: mountain ranges have low-density roots.*

This crucial finding was 'coupled' to Earth dynamics only one hundred years later and was not explored in the continental drift hypothesis.

**1895–1915:** *The unforeseen discovery of radioactivity.*

That 'killed' the concept of progressive dissipation of the heat of the Earth, and then the correlative contraction as the mechanism for orogenic stresses. It also changed the estimation of the age of the Earth and stratas by an order of magnitude . . . All this forced further serious rethinking of geological concepts about dynamic processes shaping the Earth.

**1910:** *Frank B. Taylor, Continental Drift hypothesis.*

The real beginning of 'drifting' toward plate tectonics, still a long way to go.

**1912–1946:** *Alfred Wegener, further developed the Continental Drift hypothesis, and showed a correspondence of the geological provinces, relict mountain ranges and fossil types. Driving forces – tidal/rotation of the Earth. Single protocontinent – Pangea.*

The principal questions are considered to be, 'why do continents move?' and 'what are the driving forces?' and not yet, 'how do continents move?' and 'what is the movement mechanism?'

**1916:** *Gustaaf Adolf Frederik Molengraaff proposed mid-ocean ridges to be formed by seafloor spreading as the result of the movement of continents in order to account for the opening of the Atlantic Ocean as well as the East Africa Rift.*

The mid-ocean ridges were 're-discovered' for plate tectonics 40 years later . . .

**1924:** *Harold Jeffreys showed the insufficiency of Wegener's forces to move continents.*

Computing forces for testing a geodynamic hypothesis is one of the core principles of modern geodynamics as well! Another point to learn – opposition to the Continental Drift hypothesis using physical arguments was always strong and probably considerably delayed the theory of plate tectonics.

**1931:** *Arthur Holmes suggested that thermal convection in the Earth's mantle can drive continental drift.*

This crucial idea answered a question about driving forces, but not about the movement mechanisms. It was known from seismic studies, that the Earth's mantle is in a solid state and elastic deformation does not allow thousands of kilometres of motion of the continents.

**1935:** *N. A. Haskell established the fluid-like behaviour of the mantle (viscosity $10^{20}$ Pa s) based on the analysis of beach terraces in Scandinavia and the existence of post-glaciation rebound.*

Actually, this was also established earlier from inferring crustal roots. The question about the physical mechanisms of solid-state mantle deformation remains open.

**1937:** *Alexander du Toit suggested the existence of two protocontinents – Laurasia and Gondwanaland, separated by the Tethys ocean.*

This is a really dramatic story: geologists were continuously developing and supporting the Continental Drift hypothesis, but the general idea of large lateral displacements of continents was continuously rejected by geophysicists.

**1950s:** *Improved understanding of the worldwide network of mid-ocean ridges during the extensive exploration of the seafloor.*

Evidence is critically growing in line with Molengraaff's ideas . . .

**1950s:** *Finding mechanisms of solid-state creep of crystalline materials applicable, for example, for the flow of ice in glaciers.*

The answer to the second crucial question was finally found in material science!

## Breakthrough! The Great 1960s have started!

**1960s:** *Palaeomagnetic studies, the finding of regular patterns of magnetic anomalies on the sea floor.*

**1962:** *Harry Hess suggested that the seafloor was created at the axis of the ridge.*

In fact, this was a refinement of the Molengraaff's hypothesis.

**1965:** *B. Gordon proposed the quantitative link between solid-state creep and mantle viscosity.*

**1968:** *Jason Morgan formulated the basic hypothesis of Plate Tectonics (mosaic of rigid plates in relative motion with respect to one another as a natural consequence of mantle convection).*

**1968:** *Isacks and co-workers attributed earthquakes, volcanoes and mountain building to plate boundaries.*

**1967–1970:** *Development and broad acceptance of Plate Tectonics.*

Before this time, continental drift was always opposed by geophysicists based on the rigidity of the solid elastic mantle and the 'absence' of physical mechanisms allowing horizontal displacements of thousands of kilometres for continents.

The crucial point that was finally understood by the geological community is that both viscous (i.e., fluid-like) and elastic (i.e., solid-like) behaviour is a characteristic of the Earth depending on the timescale of deformation: the Earth's mantle, which is elastic on a human timescale is viscous on geological timescales (>10 000 years) and can be strongly internally deformed due to solid state creep. There is an amazing substance demonstrating a similar 'dual' viscous–elastic behaviour. This is silicon putty or 'silly putty' which is frequently used as an analogue of rocks in experimental tectonics. It deforms like clay in the hands, but when dropped on the floor it jumps up like a rubber ball (see animation **Silly_putty.mpg**).

Plate tectonics has largely established both a conceptual and a physical basis of geodynamics. The next rapid development of numerical methods of continuum mechanics in this field is the logical consequence of both theoretical and technological progress. Numerical modelling is a necessary tool for geodynamics since tectonic processes are too slow and too deep in the Earth to be observed directly. The snapshot-like history of 2D/3D numerical geodynamic modelling (1D models appeared even earlier!) looks as follows (partly subjective literature-web-search-based view, more details on this issue can be found in several overviews on mantle convection modelling: Richter, 1978; Schubert, 1992; Bercovici, 2007):

**1970:** *First 2D numerical models of subduction (Minear and Toksoz*, 1970*)*. Exactly the time when the 'Plate Tectonics Era' had just started! The first subduction model was purely thermal, with a prescribed velocity field corresponding to the downgoing slab inclined at 45°.

**1971:** *First 2D mantle thermal convection models (Torrance and Turcotte*, 1971*)*. This paper discussed possible implications of mantle convection with temperature-dependent viscosity for continental drift. Thermomechanical models based on the stream function formulation for the mechanical part were explored. A rectangular model domain, with a temperature-dependent viscosity and resolution up to 22 × 16 nodal points was used.

**1972, 1978:** *First 2D numerical (finite-element) models of salt domes dynamics (Berner* et al., 1972; *Woidt*, 1978*)*. Before that, geodynamic modelling studies of crustal diapirism used analytical and analogue modelling approaches. Paper by Woidt (1978) pointed out inconsistency of the numerical approach used by Berner *et al.* (1972).

**1977–1980:** *First 2D mantle thermal-chemical convection models (Keondzhyan and Monin*, 1977, 1980*)*. A binary stratified medium was used to study the effects of compositional layering on mantle convection.

**1978:** *First numerical models of continental collision (Daignières* et al., 1978; *Bird*, 1978*)*. Mechanical models exploring the finite-element approach.

**1985–1986:** *First 3D spherical mantle convection models (Baumgardner*, 1985, *Machetel* et al., 1986*)*. The first 3D models were spherical and not Cartesian as one would expect. Also, for some reason, the first paper appeared in the *Journal of Statistical Physics*, which is not really a geophysical journal . . .

**1988:** *First 3D Cartesian mantle convection models (Cserepes* et al., 1988; *Houseman*, 1988*)*.

Since the 1980s, numerical geodynamic modelling has been developing very rapidly in terms of both the number of various applications and numerical techniques explored. Geodynamic modelling now stands as one of the most dynamic and advanced fields of Earth Sciences.

## A few words about programming and visualisation

In this book MATLAB is used for the exercises and for visualisation. This is a good language of choice for people starting with modelling as it allows both easy computing and visualisation. C and FORTRAN are often used for advanced studies that involve usage of supercomputers and computer clusters. In these studies, visualisation is mostly done as a post-processing step that allows independent use of specialised visualisation packages. In our short book, we are more interested to see results instantaneously, during computations. In addition, MATLAB greatly simplifies the solving of system of linear equations which is the core of numerical modelling.

In this book we will consider many example programs, since learning *to write programs* (*and not just using them*) is an essential part of numerical geodynamic modelling. There are nine important programming rules (which I call *Bug Rules*) which you should follow when writing your own programs.

**Bug Rule 1:** ***Think before programming!*** Think carefully about the algorithm of your new code and the most efficient way of making modifications to your old code – you will then develop the program faster and more efficiently and will not need too much code re-thinking and re-writing.

**Bug Rule 2:** ***Comment!*** Making comments in the code is essential to enable the code to be used, debugged and modified correctly. The ratio between comment lines and program lines in a good numerical code is larger then 1:1. Do not be lazy, explain every program line – this will save you a lot of time afterwards!

**Bug Rule 3:** ***Programming makes bugs!*** We always introduce *bugs* (i.e. programming errors) while writing a code. We typically introduce at least one bug when we modify one single line and we have to test the modified code until we find the bug!

**Bug Rule 4:** ***Programming means debugging!*** Be prepared that only 1% of the time will be spent on programming and 99% of your time will be for debugging.

**Bug Rule 5:** ***Most difficult bugs are trivial ones!*** There are three types of the most common bugs:

- errors in index (90% of your bugs!), e.g. y = x(i, j) + z(12) instead of y = x(j, i) − z(2)
- errors in sign, e.g. y = x + z instead of y = x−z or y = 1e − 19 instead of y = 1e + 19
- errors in order of magnitude, e.g. y = 0.0831 instead of y = 0.00831.

Don't be surprised that finding these 'trivial' bugs will sometimes be very difficult (we simply don't see them) and will take a lot of time – this is normal.

**Bug Rule 6:** ***If you see something strange– there is a bug!*** Be suspicious, do not ignore even small strange things and discrepancies that you see when computing with your code – in 100% of cases you will find that a bug is the cause. Never try to convince yourself (although this is what we typically tend to do) that a single last digit discrepancy in results with the previous version of the code is due to computer accuracy – it is due to either old or new bugs!

**Bug Rule 7:** ***Single bug can ruin 10 000-lines code!*** We should really be motivated to carefully debug and test codes. Don't think that one single small error in the code can be ignored – it will spoil results of months of calculations.

**Bug Rule 8:** ***Wrong model looks beautiful and realistic!*** Often erroneous models do not look bad or strange and some of them are really beautiful. Therefore, be prepared that of the numerical modelling results you like, some are actually wrong . . .

**Bug Rule 9:** ***Creating a good, correct and nicely working code is possible!*** This is what should motivate us to follow the eight previous rules!

### *Units*

In this book, the metre-kilogram-second (MKS) system is used in all basic equations as a standard, with only occasional specified deviations toward other conventional units widely used in geosciences (kbar, °C etc.).

### How to use this book

Once again, this is a textbook which is primarily aimed at people inexperienced with numerical methods. Therefore, it is organised in a way that, after my learning and teaching experience, provides the easiest path for learning the basics of continuum mechanics and numerical geodynamic modelling. Follow it from one chapter to the next and do all the exercises. Do all the programming by yourself and study code examples ONLY when you are stuck or unsure what to do (all 67 quoted MATLAB codes are provided with this book). The complexity of the programming exercises gradually increases from one chapter to the next, introducing more and more complex aspects of continuum mechanics and numerical modelling. Just trust this way and *don't give up*!

## Programming exercises and homework

### Exercise Introduction.1

Open MATLAB and use it for the first time. Study the following (use MATLAB Help to read about various functions and operations):

(a) Defining variables, vectors and matrixes
(b) Using mathematical functions (+, −, *, .*, /, ./, ^, .^, *exp, log10*, etc.)
(c) Opening/closing text files and loading/writing data from/to them (*fopen, fclose, fscanf, fprintf*)
(d) Plotting of data in 2D and 3D (*figure, plot, pcolor, surf, xlabel, ylabel, shading, light, lighting, axis, colorbar*)
(e) programming loops (*for, while, end*) and conditions (*if, else, end, switch, case*, &&, ||, ==, ~=, >, <, >=, <= etc.)

### Exercise Introduction.2

Write your first MATLAB code for visualising *sin, cos* functions in 2D (*plot, pcolor, contour*) and 3D (*surf, light, lighting*). An example is in **Visualisation_is_important.m**.

# 1

# The continuity equation

**Theory:** Definition of a geological medium as a continuum. Field variables used for the representation of a continuum. Methods for definition of the field variables. Eulerian and Lagrangian points of view. Continuity equation in Eulerian and Lagrangian forms and their derivation. Advective transport term. Continuity equation for an incompressible fluid.
**Exercises:** Computing the divergence of velocity field in 2D.

## 1.1 Continuum – what is it?

What we should understand from the very beginning is that geodynamics considers major rock units, such as the Earth's crust and mantle as *continuous geological media*. *Continuity* of any medium implies that, on a macroscopic scale, the material under consideration does not contain *mass-free voids or gaps* (there can indeed be pores or cavities but they are also filled with some continuous substances). Different physical properties of a continuum may vary at every geometrical point and we thus need a *continuous description*. In *continuum mechanics*, the physical properties of a continuum (*field properties*) are described by *field variables* such as pressure, temperature, density, velocity, etc. There are three major types of field variables:

*scalars* (e.g., pressure, temperature, density),
*vectors* (e.g., velocity, mass flux, heat flux),
*tensors* (e.g. stress, strain, strain rate).

Field variables can be represented in a *fully continuous* manner (analytical expressions, Fig. 1.1(a)) or in a *discrete-continuous* way (by arrays of values which characterise selected *nodal* geometrical points, Fig. 1.1(b–d)). In the latter case,