Introduction

Theory: What is this book? What this book is not. Get started. Seven golden rules for learning the subject. Short history of geodynamics and numerical geodynamic modelling. Few words about programming and visualization. Ten programming rules.
Exercises: Starting with MATLAB. Visualization 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 yours!

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, look at Chapters 12–21 where some advanced numerical techniques and model examples are discussed. Then you can decide if you wish to read about the technical details presented in these and other 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 human scales of direct observation are extremely limited in both time and space (depth) and since rapid progress

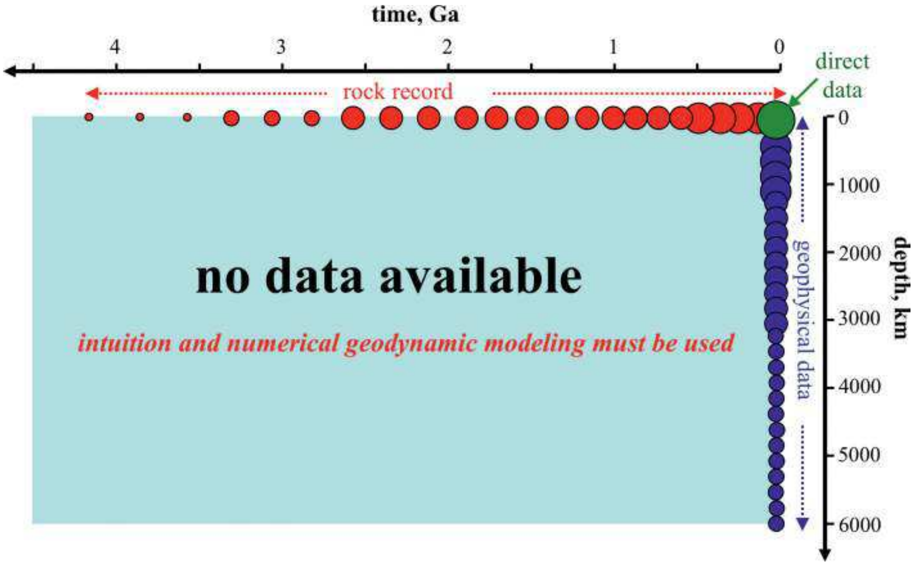

Fig. 1. Time-depth diagram presenting the availability of data for constraining geodynamic evolution of the Earth (Gerya, 2014b). The size of data points reflects the abundance of available data. This is obviously a simplified view since for a spherical Earth such a diagram should be four dimensional.

in computer technology offers every day new and exceptional possibilities to explore sophisticated mathematical models. This is true in every discipline, and even industrial applications.

Numerical geodynamic modelling naturally 'compensates' for the fundamental unavailability of data needed for constraining the evolution of the Earth's interior and surface over time, which is the subject of geodynamics. The following simple exercise explores this subject in the context of the availability of data. Let us imagine an ideally symmetrical Earth with physical properties (density, viscosity, temperature, etc.) as functions of depth and time. A simple two-dimensional time-depth diagram covering the Earth's entire history and its interior will thus be a schematic representation of the subject of geodynamics (Fig. 1). The entire diagram should then be covered by data points characterizing the physical state of the Earth at different depths, ranging from 0 to 6000 km, and for different moments of geological time, ranging from 0 to around 4.5 billion years ago. However, the unfortunate fact for geodynamics is that observations for such systematic coverage are only available along the two axes of the diagram: geophysical data for the present-day Earth structure and the historical record in rocks formed close (typically within a few tens of kilometres) to the Earth's surface. The rest of the diagram is thus fundamentally devoid of observational data, so we have to rely on something else. What else can we use? Scientific intuition based on geological experience and modelling based on fundamental laws of continuum mechanics! However, our intuition cannot always be suitable for geodynamical processes that are completely beyond human scales in time (a few years) and space (a few metres). We have to accept that some of these processes could look completely counterintuitive to us. The ways in which various geodynamic processes interact with each other can also be very difficult to conceive using only scientific intuition. This is why *intuition in geodynamics should be – must be – assisted and calibrated by modelling*. In a way, modelling helps train our intuition for very deep and very slow geological processes that cannot be observed directly. Another role of modelling is the quantification of geodynamic processes based on the sparse array of available observations. Consequently, the systematic use of numerical modelling is crucial to develop, test, and quantify geodynamic hypotheses – and perhaps most questions about the Earth.

At present, numerical modelling in geosciences is widely used for both testing and generating hypotheses, thereby strongly pushing geology from an observational, intuitive to a deductive, predictive natural science. Geo-modelling and geo-visualization 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 pushes 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 not affordable for persons with traditional geological background and should be performed by mathematicians.

I was thinking 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.' – did I think 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:

- derivatives and
- linear algebra.

Most of this '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,
algorithmic THINKING (ability to 'translate' generic tasks into code algorithms),
usual MATH,
clear EXPLANATIONS,
regular EXERCISES.

Motivation and algorithmic thinking are 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. 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 energy).

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. Many of these books are, however, written for physicists and engineers and need effort to be ‘digested’ by people with a traditional geological background. The situation has improved recently after several books written by experienced geodynamicists have appeared on the market (Gerya, 2010a; Ismail-Zadeh and Tackley, 2010; Simpson, 2017; Morra, 2018).

Golden Rule 5. ***Repeat the 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 understanding the structure of the different PDEs. This book, by the way, is full of such trivial detailed transformations – follow them carefully!

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

Without proper visualization of results, almost nothing can be done with numerical modelling (Fig. 2). Modellers often spend more time on visualization than on computing and programming.

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

This is the most efficient way of learning. In numerical geodynamic modelling, many small numerical know-hows exist. They are extremely important, but rarely discussed in publications (in contrast to this book ☺). Indeed, *do not rely solely on asking* – first try hard to find your own answer to the problem you want to solve numerically.

Short history of geodynamics and numerical geodynamic modelling

The numerical modelling approaches discussed in this book are adopted for solving *thermomechanical* geodynamic problems. Geodynamics is dynamics of the Earth – a

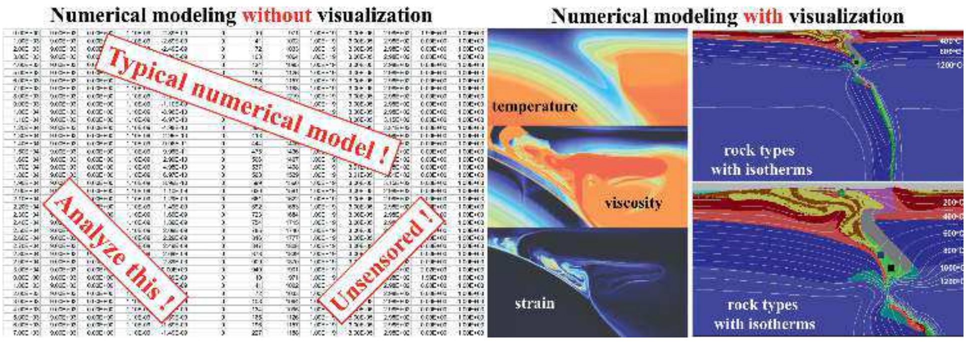

Fig. 2. Rule 6. Visualization is important!

core geological subject that has been 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 and rapidly 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, 2014). According to this introduction and further literature search, the following steps were notable historically 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 before we could start to interpret this similarity.

1665: *Athanasius Kircher, in his two-volume 'Mundus subterraneus', probably the first printed work on geophysics and volcanology, 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 mantle convection.

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

This began our understanding of the Earth as a hot layered planetary body. One really needed vision to guess this around 300 years ago!

Later part of the nineteenth century: *The fluid-like behaviour of the Earth's mantle was established, 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 the correlative contraction, as the mechanism for orogenic stresses. It also changed 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 formulated the Continental Drift hypothesis.*

This was 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 – Pangaea.*

The principal question is 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 that mid-ocean ridges are 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 that Wegener's forces were insufficient for moving continents.*

Computing forces for testing a geodynamic hypothesis is one of the core principles of modern geodynamics as well! Another point to learn is that opposition to the continental drift hypothesis using physical arguments was always strong and probably strongly 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 questions about the movement mechanisms. It was known from seismic studies that the Earth's mantle is in a solid state and that 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 had also been established earlier from inferring crustal roots. The question about the physical mechanisms of solid-state mantle deformation remained 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: *Understanding of the world-wide network of mid-ocean ridges was improved during extensive exploration of the seafloor.*

Evidence is critically growing in line with Molengraaf's ideas …

1950s: *Mechanisms of solid-state creep of crystalline materials were discoved which were applicable, for example, to the flow of ice in glaciers.*

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

Breakthrough! The great 1960s started!

1960s: *Paleomagnetic studies led to the finding of regular patterns of magnetic anomalies on the seafloor.*

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

In fact, this was a refinement of Molengraaf'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: *This saw the development and broad acceptance of plate tectonics.*

Before this time, continental drift was opposed by geophysicists because of 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 time scale of deformation. The Earth's mantle, which is elastic on a human time scale, is viscous on geological time scales (>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.m1v**).

Plate tectonics 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. 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 of mantle convection modelling: Richter, 1978; Schubert, 1992; Bercovici, 2007).

1970: *First 2D numerical models of subduction (Minear and Toksöz,* 1970*).*

Exactly at the time when the 'plate tectonics era' had just started! The first subduction model was thermo-kinematic, with a prescribed velocity field corresponding to a down-going 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 of up to 22 × 16 nodal points was used.

1972, 1978: *First 2D numerical (finite element) models of salt dome dynamics (Berner et al.,* 1972*; Woidt,* 1978*).*

Before this, geodynamic modelling studies of crustal diapirism used analytical and analogue modelling approaches. The paper by Woidt (1978) pointed out the inconsistency of the numerical approach used by Berner et al. (1972).

1977–1980: *First 2D thermal-chemical mantle 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 (Bird,* 1978*; Daignières et al.,* 1978*).*

Mechanical models explored the finite element approach.

1983: *First numerical models of subduction initiation (Matsumoto and Tomoda,* 1983*).*

Remarkable geodynamic modelling ahead of its time! The numerical solution was based on stream function formulation combined with marker-in-cell technique and free surface implementation based on the 'sticky water' approach, which became widespread *two decades later*.

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 applications and the numerical techniques explored. In the last decade, several textbooks on numerical geodynamic modelling have been published (Gerya, 2010a; Ismail-Zadeh and Tackley, 2010; Simpson, 2017; Morra, 2018), which make it more accessible for geoscientists and help in teaching it to students. At present, geodynamic modelling stands as one of the most dynamic, cross-disciplinary and advanced fields of modern Earth sciences.

Few words about programming, visualization and debugging

In the frame of this book MATLAB is used for the exercises and for visualization. This is a good language of choice for people starting with modelling as it allows both easy computing and visualization. C and FORTRAN are often used for advanced studies that involve usage of supercomputers and computer clusters. In these studies, visualization is mostly done as a post-processing step that allows independent use of specialized visualization packages. In our short course, we are more interested in seeing results instantaneously, during computations. In addition, MATLAB greatly simplifies the solving of systems of linear equations, which is the core of numerical modelling. Another convenient programming language with growing popularity in geodynamics is PYTHON (Morra, 2018).

In this course, 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 ten important programming rules (which I call *Bug Rules*), which you may want to 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 spent on debugging.

Bug Rule 5: ***Nice looking codes are often more difficult to debug!*** Do not try to write nice looking codes; try to write codes that are easy to debug! Use the most simple and explicit code logic and structure. Be very pragmatic; do not make changes to previously debugged code sections unless absolutely necessary. Go for important code changes only; do not 'fight' for better looking code structure or minor improvements of computational efficiency.

Bug Rule 6: ***Bugs that are the most difficult to find are trivial ones!*** There are three types of 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.

Do not be surprised that finding these 'trivial' bugs will sometimes be very difficult (we simply tend to overlook them) and will take a lot of time – this is normal.

Bug Rule 7: ***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 8: ***A single bug can ruin a 10 000-line code!*** We should really be motivated to carefully debug and test codes. Do not think that one single small error in the code can be ignored – it will spoil the results of months of calculations.

Bug Rule 9: ***A 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 10: ***Creating a good, correct and nicely working code is possible!*** This is what should motivate us to follow the nine previous rules!

Many years of correcting students' codes made me convinced that there is only one robust (although not really elegant and efficient) way of finding bugs in a code: write two independent versions (i.e., without copy-pasting) of the same code (preferably by two different people) and compare computational results for well controlled conditions. If the results are different – there is at least one bug in at least one of the two codes. Then, try to copy-paste routines from one code version to the other until the results become identical. This helps to find routines that produce different results and to clarify reasons (bugs) for the discrepancy. Experience shows that it is very unlikely that two independent code versions will have identical bugs (even if both are written by the same person). Adding more code versions (and people) to the 'pool' will further help debugging.

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 organized in a way that, according to my personal 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 MATLAB codes quoted in the text are provided with this book, see the Appendix). 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

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 matrices.
(b) Using mathematical functions (+, -, *, .*, /, ./, ^, .^, exp, log, 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 visualizing the sin and cos functions in 2D (*plot, pcolor, contour*) and 3D (*surf, light, lighting*). An example is in **Visualisation_is_important.m**.