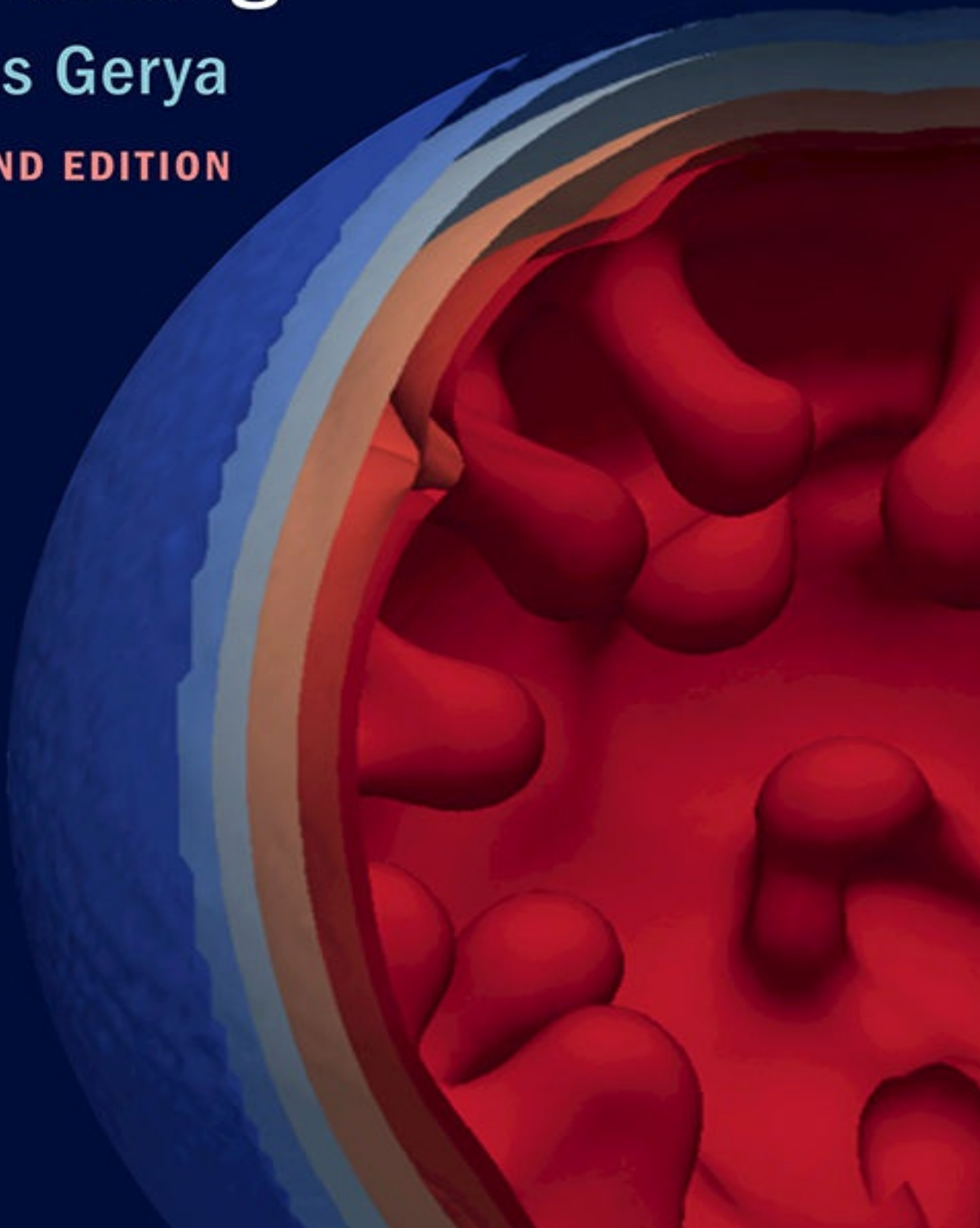
INTRODUCTION TO
Numerical Geodynamic Modelling

Taras Gerya

SECOND EDITION



INTRODUCTION TO NUMERICAL GEODYNAMIC MODELLING

This hands-on introduction to numerical geodynamic modelling provides a solid grounding in the necessary mathematical theory and techniques, including continuum mechanics and partial differential equations, before introducing key numerical modelling methods and applications. Fully updated, this second edition includes four completely new chapters covering the most recent advances in modelling inertial processes, seismic cycles and fluid-solid interactions, and the development of adaptive mesh refinement algorithms. Many well-documented, state-of-the-art visco-elasto-plastic 2D models are presented, which allow robust modelling of key geodynamic processes. Requiring only minimal prerequisite mathematical training, and featuring over 60 practical exercises and 90 MATLAB examples, this user-friendly resource encourages experimentation with geodynamic models. It is an ideal introduction for advanced courses and can be used as a self-study aid for graduates seeking to master geodynamic modelling for their own research projects.

TARAS GERYA is Professor in the Department of Earth Sciences at the Swiss Federal Institute of Technology (ETH-Zürich). He is an expert in numerical geodynamic modelling, with his current research focusing on subduction and collision processes, ridge-transform oceanic spreading patterns, intrusion emplacement into the crust, generation of earthquakes, fluid and melt transport in the lithosphere, Precambrian geodynamics, formation of terrestrial planets and evolution of life. In 2008 he was awarded the Golden Owl Prize by ETH students for his teaching on continuum mechanics and numerical modelling.

"A great introduction to computational geodynamics with vivid examples, hands-on exercises and step-by-step derivations of formulas. Even better than the first edition."

– Dr Sascha Brune, *GFZ Potsdam*

"This book is so much more than an introduction to geodynamic modelling. Taras Gerya opens the world of geodynamic experiments by taking the reader through a carefully designed set of hands-on programming exercises that will convince you that modelling is not terribly complicated, but a process to logically follow through. Go ahead and get started!" – Dr Susanne Buiter, *Geological Survey of Norway*

"This comprehensive textbook challenges all solid Earth scientists to give geodynamic modelling a try in a hands-on, empowering style. The new edition covers even more ground, including cutting-edge topics. A great achievement, and the community will be the better for it." – Professor Thorsten Becker, *University of Texas at Austin*

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Preface to the second edition

The main reason for writing this second edition is the rapid recent progress in the field of numerical geodynamic modelling, which is one of the most dynamic and fast growing fields of the modern Earth sciences. Since the publication of the first edition in 2010 (almost a decade ago . . .), several important research directions have become very prominent and advanced in computational geodynamics, such as investigation of coupled solid-fluid processes, coupling of geodynamic evolution to surface processes, modelling of seismic cycles at plate boundaries, development of adaptive grid refinement methods and free surface stabilization approaches, elaboration of more accurate continuity-based Lagrangian advection algorithms, development and broad application of new efficient 3D visco-elasto-plastic highly parallelized numerical modelling tools etc. In order to account for some of these exciting novelties, I both significantly revised some of the previously published chapters (especially numerical modelling of advection processes in Chapter 8 and numerical treatment of visco-elasto-plastic materials in Chapters 12 and 13) and added four new chapters focusing on recent numerical advances in

- modelling of inertial processes (Chapter 14),
- modelling of seismic cycles (Chapter 15),
- modelling of coupled fluid-solid processes (Chapter 16) and
- development of adaptive mesh refinement algorithms (Chapter 17).

As in the first edition, a single relatively simple numerical modelling method (combination of staggered finite differences with marker-in-cell techniques, SFD+MIC) and MATLAB programming are used uniformly throughout this textbook. I hope you will enjoy this new edition!

Acknowledgements

In relation to the first and second editions of this book I would like to acknowledge many people and I will try to do this in chronological order. I am grateful to my wife Irina for inspiration and support. I am grateful to my first supervisor Alexander Nozhkin for giving me a chance to start my scientific career in 1984. I am grateful to my PhD supervisor and good friend Leonid Perchuk (1933–2009) for suggesting that I start with numerical modelling in 1995 (a long time ago, indeed, but I feel like it was yesterday). I am grateful to Alexander Simakin for explaining to me in a few words what numerical modelling is about, when I had just started to learn it and was really puzzled what to do with all these partial differential equations written in textbooks (he told me that I simply have *to compose and solve together as many linear equations as I have unknowns* and this is really the main idea behind numerical modelling). I am grateful to Roberto Weinberg and Harro Schmeling for their excellent paper on polydiapirs, published in 1992, which introduced me to the marker-in-cell techniques when I had just started. I am grateful to Alexey Polyakov for suggesting that I use upwind differences for solving the temperature equation when I was programming my first themomechanical code. I am grateful to Walter Maresch and Bernhard Stöckhert for cooperating with me on modelling of subduction processes, which is a challenging topic and stimulated a lot of my code developments. I am grateful to David Yuen – my co-author in many important numerical modelling papers – for our long-term joint work and friendship (after we met in 2001 at the AGU Fall meeting in San Francisco) and for many great suggestions concerning this book. I am grateful to Paul Tackley for telling me about the fully staggered grid in 2002 (I was using a half-staggered grid before that time) and for introducing me to multigrid in 2005 as well as for many years of our joint studies and good suggestions concerning this book. I am grateful to Jean-Pierre Burg for inviting me to ETH-Zürich and cooperating with me on challenging modelling projects (which again triggered many code developments) and for being a very careful and constructive first reader of the initial version of this book. I am grateful to Yuriy Podladchikov for many stimulating discussions, continuous healthy criticism and challenging suggestions (for example, adding elasticity and plasticity to my codes that 'spoiled' six months of my life in 2004). I am grateful to Boris Kaus for arguing and discussing numerics with me, which we both like, and for great detailed comments and suggestions on the initial version of this book. I am grateful to James Connolly for fruitful work on coupling of

thermodynamics and phase petrology with thermomechanical experiments (what I call petrological-thermomechanical numerical modelling). I am very grateful to David May for creative checking of both the first and the second editions of this textbook and for giving many good hints about the content. I am grateful to my colleague and friend Evgenii Burov (1963–2015) for our great cooperation in the field of high-resolution 3D numerical geodynamic modelling, which unfortunately stopped very sadly in 2015. I am very grateful to Viktoriya Yarushina for her invaluable help with the chapter on solid-fluid coupling and to Anton Popov for the generous sharing of his new 3D elastic stress rotation algorithms. I am grateful to Tobias Keller for his detailed and insightful comments on the hydro-thermomechanical modelling chapter. I am grateful to Alexey Perchuk for our long-term friendship, exciting discussions and fruitful cooperation in the field of petrology and geodynamic modelling. I am grateful to my son Bogdan for computer and graphic assistance, to my parents Lyudmila and Viktor (1927–2015), my brother Artem and my entire family for moral support. I am grateful to all my students and co-authors for their bright ideas and great work done together. Finally, I am grateful for the generous support of my numerical modelling projects by Alexander von Humboldt foundation research fellowships and by many ETH, SNF and EU research grants.

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

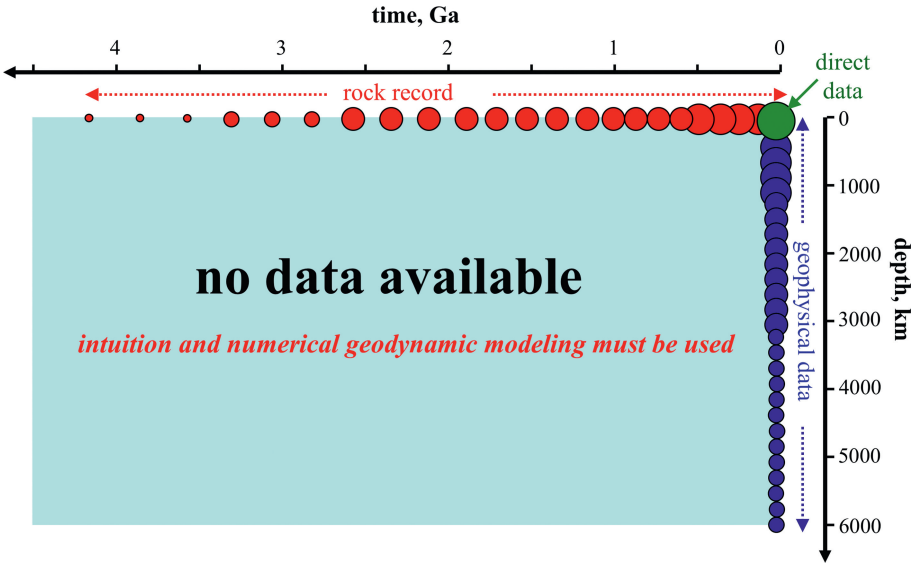

Fig. 1. Time-depth diagram presenting the availability of data for constraining geodynamic evolution of the Earth (Gerya, 2014b). The size of data points reflects the abundance of available data. This is obviously a simplified view since for a spherical Earth such a diagram should be four dimensional.

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

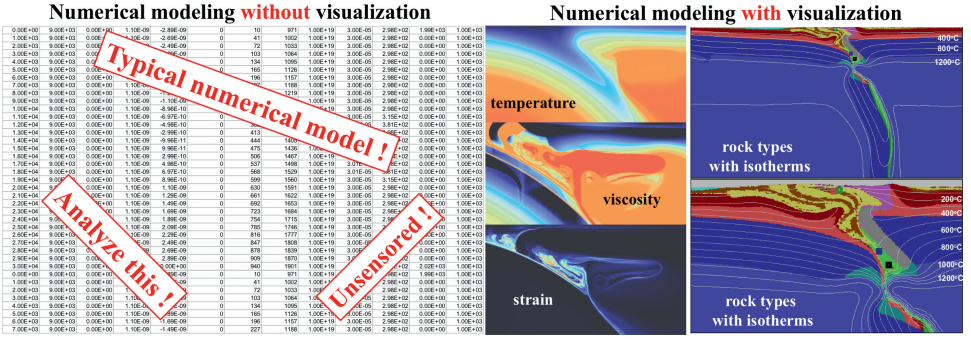

Fig. 2. Rule 6. Visualization is important!

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**.

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 derivations. Advective transport term. Continuity equation for an incompressible fluid.
Exercises: Computing the divergence of a 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. 1.1a) or in a *discrete-continuous* way (by arrays of values which characterize selected *nodal* geometrical points, Fig. 1.1b–d). In the latter case, various linear and non-linear *interpolation* rules are used to calculate values of field variables between the nodal points.

Continuity also implies that displacements of different portions of the medium are not fully independent. These displacements must proceed without creating macroscopic voids and gaps: if some rocks are displaced *from* a certain area (for example due to tectonic

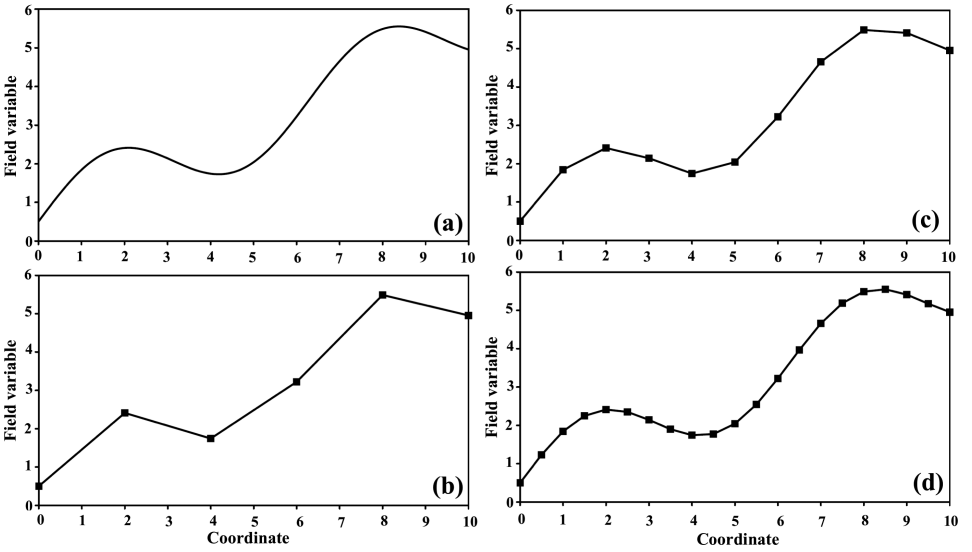

Fig. 1.1. Continuous (a) and discrete-continuous (b)–(d) representations of a field variable as a function of coordinates. Note that in the case of the discrete-continuous representation with linear interpolation between nodal points, the representation accuracy notably increases with increasing number of nodal points (compare a with b, c and d).

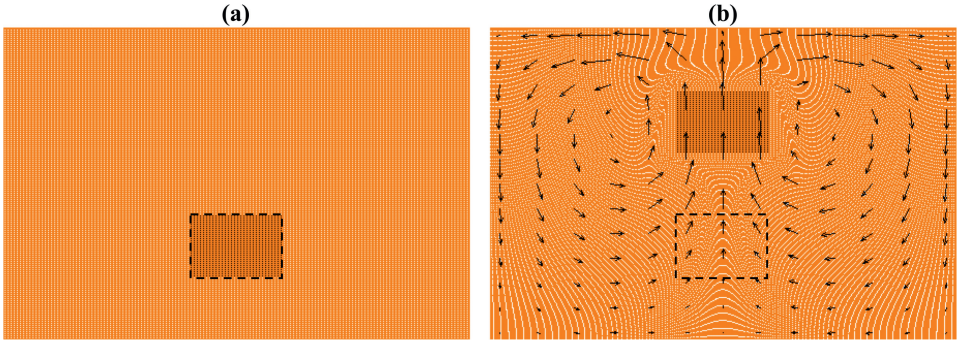

Fig. 1.2. Example of the deformation of a continuous medium (white dots) due to the buoyant rise of a rigid block (black dots): (a) initial stage, (b) final stage with the corresponding velocity field indicated by arrows. Note that no voids are formed where the block was initially located (dashed contour). Individual black and white dots in (a) and (b) correspond to different Lagrangian points displaced by the flow. Diagrams are computed numerically with the code developed by Gerya and Yuen (2003a), and an animation is shown in the file **Continuity.ppt** associated with this chapter.

extrusion), other rocks must come *into* this area and substitute the displaced fragment (Fig. 1.2). In a way, this type of continuous behaviour is very similar to that of water or, generally, any fluid which can be described with *fluid mechanics* (e.g. Landau and Lifshitz, 1987; Kundu, and Cohen, 2002). Since on long time scales rocks behave like slowly

creeping fluids, geodynamic processes in the Earth's mantle, as for example mantle convection, are often referred to as processes of *geophysical fluid dynamics*.

1.2 Continuity equation

Our qualitative, intuitive understanding of continuity can, indeed, be transformed into a quantitative mathematical formalism. This formalism is widely used in numerical geodynamic modelling in the form of a *continuity equation*, which describes the *conservation of mass* during the displacement of a continuous medium. Let us write this equation and try to understand its structure in detail.

The first thing that we have to learn is that the form of the mass conservation equation (and many other *time-dependent* conservation equations) can be either *Eulerian* or *Lagrangian* depending on the nature of the geometrical point for which this equation is written.

The Eulerian continuity equation is written for an *immobile* or fixed point in space; it has the form

$$\frac{\partial \rho}{\partial t} + \mathrm{div}(\rho \vec{v}) = 0. \tag{1.1a}$$

Or, in a slightly different symbolic notation often used in continuum mechanics,

$$\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho \vec{v}) = 0, \tag{1.1b}$$

where $\partial/\partial t$ is the Eulerian time derivative; ρ is the local density, which characterizes the amount of mass per unit volume (kg/m^3); $\vec{v}$ is local velocity (m/s) and div() or $\nabla \bullet$ denotes the divergence operator. The divergence is a scalar function of a vector field, and is defined as follows:

$$\text{in one dimension (1D)} \quad \mathrm{div}(\vec{v}) = \frac{\partial v_x}{\partial x}, \tag{1.2a}$$

$$\text{in two dimensions (2D)} \quad \mathrm{div}(\vec{v}) = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y}, \tag{1.2b}$$

$$\text{in three dimensions (3D)} \quad \mathrm{div}(\vec{v}) = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}, \tag{1.2c}$$

where x, y, and z are Cartesian coordinates and v_x, v_y and v_z are components parallel to the respective coordinate axes of the velocity vector $\vec{v}$ (Fig. 1.3). In simple words, the divergence of a vector in a given point is positive when the surrounding vector field is directed predominantly outward of the point (divergent flow, Fig. 1.4a) and is negative when this field is directed predominantly toward the point (convergent flow, Fig. 1.4b).

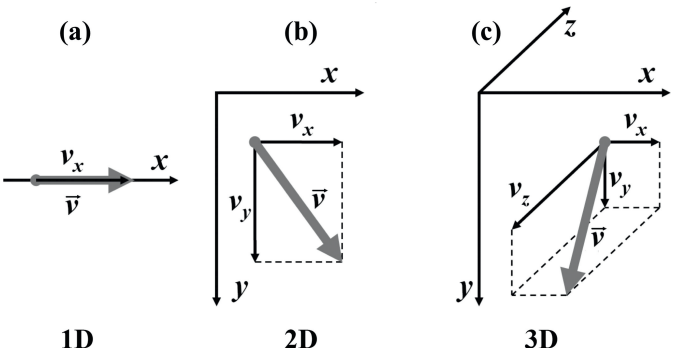

Fig. 1.3. Components of a local velocity vector $\vec{v}$ (grey arrow) in one (a), two (b), and three (c) dimensions.

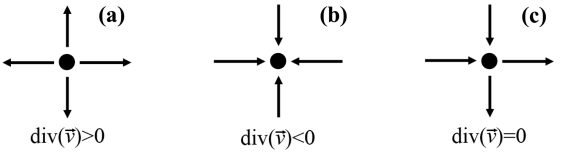

Fig. 1.4. Examples of divergent (a), convergent (b) and neutral (c) 2D velocity fields around a point.

The Lagrangian continuity equation is written for a *moving* point of reference; it has the form

$$\frac{D\rho}{Dt} + \rho \mathrm{div}(\vec{v}) = 0, \tag{1.3a}$$

or

$$\frac{D\rho}{Dt} + \rho \nabla \bullet \vec{v} = 0, \tag{1.3b}$$

where D/Dt is the Lagrangian time derivative and the other parameters were explained before (see Eq. 1.1).

1.3 Eulerian and Lagrangian points – what is the difference?

Understanding the difference between Eulerian and Lagrangian points is *fundamental* for continuum mechanics. A Lagrangian point is strictly connected to a single material point and is moving with this point. Therefore, the same material point is always found in a given Lagrangian point independent of the moment of time. For this reason, the Lagrangian time

derivative of density $D\rho/Dt$ (i.e., changes in density with time in the Lagrangian point) is also called the *substantive* or *objective* time derivative. On the other hand, an Eulerian point is an immobile observation point, not related to any specific material point. Therefore, at different moments of time, different Lagrangian material points can be found at the same Eulerian point. In other words, different Lagrangian material points are *passing through* the same Eulerian observation point with time. Good analogies for an Eulerian and a Lagrangian point are respectively a fixed window and a person walking past in front of it. Many equations of continuum mechanics containing time derivatives can be written in both Eulerian and Lagrangian forms which differ from each other (e.g. Eqs. 1.1 and 1.3). Choosing either the Eulerian or Lagrangian form of an equation notably affects the method of representing *advective transport processes* (i.e. the movement of material with the flow) which will be discussed in detail in Chapter 8, together with the advantages and disadvantages of the two approaches.

1.4 Derivation of the Eulerian continuity equation

Let us now analyse the Eulerian continuity equation (Eq. 1.1), which contains both vector (velocity) and scalar (density) variables. This equation establishes the balance of mass in a small fixed observation volume. It implies, in particular, that if mass is leaving (fluxing out of) the volume (i.e., $\mathrm{div}(\rho\vec{v}) > 0$), the local density (i.e., the amount of mass per unit volume) decreases with time (i.e., $\partial\rho/\partial t < 0$).

First we need to understand that $\rho\vec{v}$ is the local *mass flux* vector

$$\rho\vec{v} = \left(\rho v_x,\ \rho v_y,\ \rho v_z\right), \tag{1.4}$$

which has the dimension of unit mass, fluxing through a unit surface, per unit time ($\mathrm{kg}/\left(\mathrm{m}^2\mathrm{s}\right)$). This definition follows from the fact that the velocity in a continuous medium can be considered as *material volume flux* (Fig. 1.5), i.e., unit volume fluxing through a unit surface per unit time ($\mathrm{m/s} = \mathrm{m}^3/\left(\mathrm{m}^2\mathrm{s}\right)$). Therefore, velocity (i.e. volume flux) multiplied by the density (i.e. mass per unit volume) gives the mass flux.

We can derive the Eulerian continuity equation by analysing material fluxes through a small, immobile, rectangular Eulerian (observation) volume of constant dimensions Δx, Δy and Δz (Fig. 1.6a). Let us assume that the initial mass of fluid in this volume is m_0. Then, the initial average fluid density (ρ_0) within this volume is

$$\rho_0 = \frac{m_0}{\Delta x\,\Delta y\,\Delta z}. \tag{1.5}$$

Mass enters the volume through the boundaries A, C and E and leaves it through the opposite boundaries B, D and F. Material fluxes affect the mass of fluid in the observation volume and after a small period of time Δt (*time increment*), this mass becomes m_1 and the average fluid density changes to the new value (ρ_1)

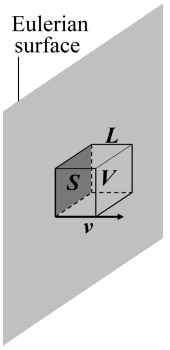

Fig. 1.5. Relationship between the flow velocity v and material volume V, passing through the element S of the immobile Eulerian surface (grey) during the time t. The relations $V = S\,L$ and $L = v\,t$ allow one to formulate velocity as the material volume flux $v = V/(St)$.

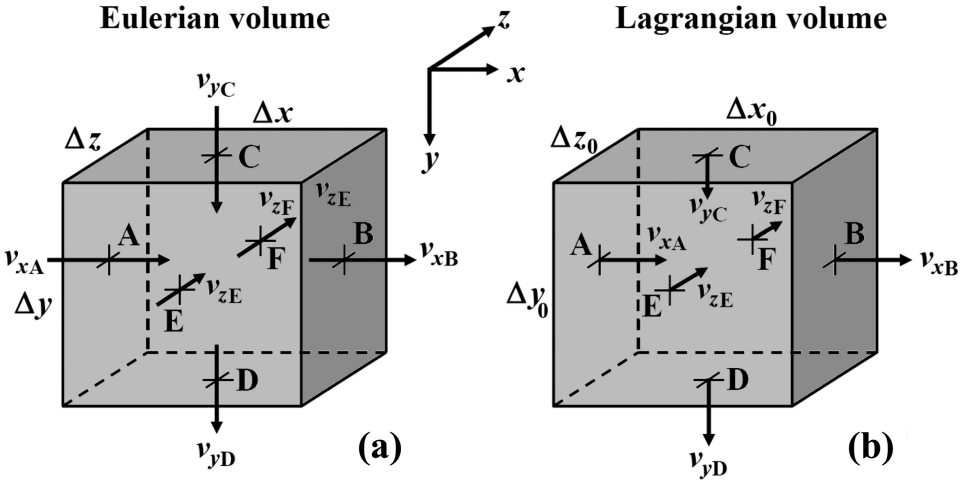

Fig. 1.6. Eulerian (a) and Lagrangian (b) elementary volumes considered for the derivation of the continuity equation. Arrows in (a) show the velocity components which are responsible for *material fluxes through* the respective boundaries (A, B, C, D, E and F). Arrows in (b) show the velocity components responsible for *moving* the respective boundaries.

$$\rho_1 = \frac{m_1}{\Delta x\,\Delta y\,\Delta z}. \tag{1.6}$$

The balance between the old (m_0) and new (m_1) masses results in the following relations:

$$
\begin{aligned}
m_1 &= m_0 + m_{in} - m_{out,}\\
m_{in} &= m_{\mathrm{A}} + m_{\mathrm{C}} + m_{\mathrm{E},}\\
m_{out} &= m_{\mathrm{B}} + m_{\mathrm{D}} + m_{\mathrm{F},}\\
m_{\mathrm{A}} &= \rho_{\mathrm{A}} v_{x\mathrm{A}} \Delta y \Delta z \Delta t,\\
m_{\mathrm{B}} &= \rho_{\mathrm{B}} v_{x\mathrm{B}} \Delta y \Delta z \Delta t,\\
m_{\mathrm{C}} &= \rho_{\mathrm{C}} v_{y\mathrm{C}} \Delta x \Delta z \Delta t,\\
m_{\mathrm{D}} &= \rho_{\mathrm{D}} v_{y\mathrm{D}} \Delta x \Delta z \Delta t,\\
m_{\mathrm{E}} &= \rho_{\mathrm{E}} v_{z\mathrm{E}} \Delta x \Delta y \Delta t,\\
m_{\mathrm{F}} &= \rho_{\mathrm{F}} v_{z\mathrm{F}} \Delta x \Delta y \Delta t,
\end{aligned}
\tag{1.7}
$$

where m_{in} and m_{out} are the incoming and outgoing masses, respectively; m_{A} to m_{F} are masses that passed through the respective boundaries during the time Δt; ρ_{A} to ρ_{F} are the densities at the respective boundaries; $v_{x\mathrm{A}}$ to $v_{z\mathrm{F}}$ are the velocity components responsible for material fluxes through the boundaries (Fig. 1.6a). If Δt is small, we can now write an approximate expression for the Eulerian time derivative of the average density in the volume as:

$$
\frac{\partial \rho}{\partial t} \approx \frac{\Delta \rho}{\Delta t} = \frac{\rho_1 - \rho_0}{\Delta t} = \frac{m_1 - m_0}{\Delta x\, \Delta y\, \Delta z\, \Delta t}. \tag{1.8a}
$$

By using Eq. (1.7) the following expression can be obtained (verify as an exercise)

$$
\frac{\Delta \rho}{\Delta t} = -\frac{\rho_{\mathrm{B}} v_{x\mathrm{B}} - \rho_{\mathrm{A}} v_{x\mathrm{A}}}{\Delta x} - \frac{\rho_{\mathrm{D}} v_{y\mathrm{D}} - \rho_{\mathrm{C}} v_{y\mathrm{C}}}{\Delta y} - \frac{\rho_{\mathrm{F}} v_{z\mathrm{F}} - \rho_{\mathrm{E}} v_{z\mathrm{E}}}{\Delta z}, \tag{1.8b}
$$

or

$$
\frac{\Delta \rho}{\Delta t} = -\frac{\Delta(\rho v_x)}{\Delta x} - \frac{\Delta(\rho v_y)}{\Delta y} - \frac{\Delta(\rho v_z)}{\Delta z}, \tag{1.8c}
$$

or

$$
\begin{aligned}
\frac{\Delta \rho}{\Delta t} + \frac{\Delta(\rho v_x)}{\Delta x} + \frac{\Delta(\rho v_y)}{\Delta y} + \frac{\Delta(\rho v_z)}{\Delta z} &= 0,\\
\Delta(\rho v_x) &= \rho_{\mathrm{B}} v_{x\mathrm{B}} - \rho_{\mathrm{A}} v_{x\mathrm{A},}\\
\Delta(\rho v_y) &= \rho_{\mathrm{D}} v_{y\mathrm{D}} - \rho_{\mathrm{C}} v_{y\mathrm{C},}\\
\Delta(\rho v_z) &= \rho_{\mathrm{F}} v_{z\mathrm{F}} - \rho_{\mathrm{E}} v_{z\mathrm{E},}
\end{aligned}
\tag{1.8d}
$$

where $\Delta(\rho v_x)$, $\Delta(\rho v_y)$ and $\Delta(\rho v_z)$ are differences in the mass fluxes in the *x, y* and *z* directions respectively (i.e. through the respective pairs of boundaries, Fig. 1.6a). Obviously, in such cases when Δt, Δx, Δy and Δz all tend to zero, the differences can be replaced by derivatives and we obtain the Eulerian continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v_x)}{\partial x} + \frac{\partial (\rho v_y)}{\partial y} + \frac{\partial (\rho v_z)}{\partial z} = 0, \tag{1.9a}$$

or

$$\frac{\partial \rho}{\partial t} + \mathrm{div}(\rho \vec{v}) = 0. \tag{1.9b}$$

1.5 Derivation of the Lagrangian continuity equation

Similarly, we can derive the Lagrangian continuity equation by analysing the motion of a small, mobile, rectangular Lagrangian (material) volume of initial dimensions Δx_0, Δy_0 and Δz_0 (Fig. 1.6b). In contrast to the fixed Eulerian volume, the amount of mass m in the moving Lagrangian volume remains constant (since this volume always contains the same material points), but the dimensions of the volume may change due to *internal* expansion/contraction processes. The initial average fluid density (ρ_0), within the volume is given by

$$\rho_0 = \frac{m}{\Delta x_0 \, \Delta y_0 \, \Delta z_0}. \tag{1.10}$$

Internal expansion or contraction affects the dimensions of the Lagrangian volume, and after a small period of time Δt, these dimensions become Δx_1, Δy_1 and Δz_1 and the average fluid density (ρ_1) changes to

$$\rho_1 = \frac{m}{\Delta x_1 \, \Delta y_1 \, \Delta z_1}. \tag{1.11}$$

We can establish the relationship between the old (Δx_0, Δy_0, Δz_0) and the new (Δx_1, Δy_1, Δz_1) dimensions of the Lagrangian volume on the basis of the relative movements of the boundaries of the volume (A, B, C, D, E, F, Fig. 1.6b), which leads to the following relations:

$$\begin{aligned} \Delta x_1 &= \Delta x_0 + \Delta t \, \Delta v_{x,} \\ \Delta v_x &= v_{x\mathrm{B}} - v_{x\mathrm{A}}, \end{aligned} \tag{1.12}$$

$$\begin{aligned} \Delta y_1 &= \Delta y_0 + \Delta t \, \Delta v_{y,} \\ \Delta v_y &= v_{y\mathrm{D}} - v_{y\mathrm{C}}, \end{aligned} \tag{1.13}$$

$$\begin{aligned} \Delta z_1 &= \Delta z_0 + \Delta t \, \Delta v_{z,} \\ \Delta v_z &= v_{z\mathrm{F}} - v_{z\mathrm{E}}, \end{aligned} \tag{1.14}$$

where Δv_x, Δv_y and Δv_z are the differences in the velocity components that correspond to the relative movements of respective pairs of boundaries (Fig. 1.6b). Taking Δt to be small, we can now write an approximate expression for the Lagrangian time derivative of the average density in the volume as

$$\frac{D\rho}{Dt} \approx \frac{\Delta\rho}{\Delta t} = \frac{\rho_1 - \rho_0}{\Delta t} = \frac{m}{\Delta x_1\ \Delta y_1\ \Delta z_1\ \Delta t} - \frac{m}{\Delta x_0\ \Delta y_0\ \Delta z_0\ \Delta t}. \tag{1.15}$$

By using the equations derived for Δx_1, Δy_1 and Δz_1 (Eqs. 1.12–1.14) the following expression can be obtained (verify as an exercise):

$$\frac{\Delta\rho}{\Delta t} = \rho_0 \frac{1 - \left(1 + \Delta t \frac{\Delta v_x}{\Delta x_0}\right)\left(1 + \Delta t \frac{\Delta v_y}{\Delta y_0}\right)\left(1 + \Delta t \frac{\Delta v_z}{\Delta z_0}\right)}{\Delta t\left(1 + \Delta t \frac{\Delta v_x}{\Delta x_0}\right)\left(1 + \Delta t \frac{\Delta v_y}{\Delta y_0}\right)\left(1 + \Delta t \frac{\Delta v_z}{\Delta z_0}\right)}, \tag{1.16a}$$

or

$$\frac{\Delta\rho}{\Delta t} = \rho_0 \frac{-\frac{\Delta v_x}{\Delta x_0} - \frac{\Delta v_y}{\Delta y_0} - \frac{\Delta v_z}{\Delta z_0} - \Delta t\left(\frac{\Delta v_x}{\Delta x_0}\frac{\Delta v_y}{\Delta y_0} + \frac{\Delta v_x}{\Delta x_0}\frac{\Delta v_z}{\Delta z_0} + \frac{\Delta v_y}{\Delta y_0}\frac{\Delta v_z}{\Delta z_0} + \Delta t \frac{\Delta v_x}{\Delta x_0}\frac{\Delta v_y}{\Delta y_0}\frac{\Delta v_z}{\Delta z_0}\right)}{\left(1 + \Delta t \frac{\Delta v_x}{\Delta x_0}\right)\left(1 + \Delta t \frac{\Delta v_y}{\Delta y_0}\right)\left(1 + \Delta t \frac{\Delta v_z}{\Delta z_0}\right)}, \tag{1.16b}$$

or

$$\frac{\Delta\rho}{\Delta t} + \rho_0 \frac{\frac{\Delta v_x}{\Delta x_0} + \frac{\Delta v_y}{\Delta y_0} + \frac{\Delta v_z}{\Delta z_0} + K_1}{K_2} = 0, \tag{1.16c}$$

where

$$K_1 = \Delta t\left(\frac{\Delta v_x}{\Delta x_0}\frac{\Delta v_y}{\Delta y_0} + \frac{\Delta v_x}{\Delta x_0}\frac{\Delta v_z}{\Delta z_0} + \frac{\Delta v_y}{\Delta y_0}\frac{\Delta v_z}{\Delta z_0} + \Delta t \frac{\Delta v_x}{\Delta x_0}\frac{\Delta v_y}{\Delta y_0}\frac{\Delta v_z}{\Delta z_0}\right)$$

$$K_2 = \left(1 + \Delta t \frac{\Delta v_x}{\Delta x_0}\right)\left(1 + \Delta t \frac{\Delta v_y}{\Delta y_0}\right)\left(1 + \Delta t \frac{\Delta v_z}{\Delta z_0}\right).$$

K_1 and K_2 are coefficients which respectively tend to *zero* and *unity* when Δt tends to zero. Obviously, in the case when Δt, Δx_0, Δy_0 and Δz_0 all tend towards zero, the differences in Eq. (1.16c) can be replaced by derivatives and taking $K_1 = 0$ and $K_2 = 1$ we obtain the Lagrangian continuity equation

$$\frac{D\rho}{Dt} + \rho\frac{\partial v_x}{\partial x} + \rho\frac{\partial v_y}{\partial y} + \rho\frac{\partial v_z}{\partial z} = 0, \tag{1.17a}$$

or

$$\frac{D\rho}{Dt} + \rho\ \mathrm{div}(\vec{v}) = 0. \tag{1.17b}$$

1.6 Comparing Eulerian and Lagrangian continuity equations: advective transport term

Let us now perform transformations of the Eulerian continuity equation (Eq. 1.1) in order to decipher its structure and to establish a relationship with the Lagrangian continuity equation (Eq. 1.3). It is convenient to decompose $\mathrm{div}(\rho\vec{v})$ using the standard *product rule* (also called *Leibniz's law*) $(u \cdot v)' = u' \cdot v + v' \cdot u$, or $\partial(uv)/\partial x = (\partial u/\partial x)v + (\partial v/\partial x)u$

$$\mathrm{div}(\rho\vec{v}) = \rho\mathrm{div}(\vec{v}) + \vec{v}\ \mathrm{grad}(\rho), \tag{1.18a}$$

or in a different symbolic notation

$$\nabla\bullet(\rho\vec{v}) = \rho\nabla\bullet\vec{v} + \vec{v}\bullet\nabla\rho, \tag{1.18b}$$

or 'deciphering' what we actually are doing in three dimensions

$$\frac{\partial}{\partial x}(\rho v_x) + \frac{\partial}{\partial y}(\rho v_y) + \frac{\partial}{\partial z}(\rho v_z) = \left(\rho\frac{\partial v_x}{\partial x} + \rho\frac{\partial v_y}{\partial y} + \rho\frac{\partial v_z}{\partial z}\right) + \left(v_x\frac{\partial \rho}{\partial x} + v_y\frac{\partial \rho}{\partial y} + v_z\frac{\partial \rho}{\partial z}\right), \tag{1.18c}$$

where $\mathrm{grad}(\rho)$ or $\nabla\rho$ is the gradient of the density ρ. The gradient is a vector function of a scalar field defined as follows:

$$\text{in one dimension (1D)} \quad \mathrm{grad}(\rho) = \left(\frac{\partial \rho}{\partial x}\right), \tag{1.19a}$$

$$\text{in two dimensions (2D)} \quad \mathrm{grad}(\rho) = \left(\frac{\partial \rho}{\partial x}, \frac{\partial \rho}{\partial y}\right), \tag{1.19b}$$

$$\text{in three dimensions (3D)} \quad \mathrm{grad}(\rho) = \left(\frac{\partial \rho}{\partial x}, \frac{\partial \rho}{\partial y}, \frac{\partial \rho}{\partial z}\right). \tag{1.19c}$$

Therefore, both $\nabla\rho$ and $\vec{v}$ in Eq. (1.18) are vectors and the *scalar product* (or *dot product*) of these two vectors (1.18c) gives the following result:

$$\text{in one dimension (1D)} \quad \vec{v}\ \mathrm{grad}(\rho) = v_x\frac{\partial \rho}{\partial x}, \tag{1.20a}$$

$$\text{in two dimensions (2D)} \quad \vec{v}\ \mathrm{grad}(\rho) = v_x\frac{\partial \rho}{\partial x} + v_y\frac{\partial \rho}{\partial y}, \tag{1.20b}$$

$$\text{in three dimensions (3D)} \quad \vec{v}\ \mathrm{grad}(\rho) = v_x\frac{\partial \rho}{\partial x} + v_y\frac{\partial \rho}{\partial y} + v_z\frac{\partial \rho}{\partial z}. \tag{1.20c}$$

Now by comparing Eqs. (1.1), (1.3) and (1.18) we can establish the relationship between the Eulerian $(\partial\rho/\partial t)$ and Lagrangian $(D\rho/Dt)$ time derivatives of density as