Geodynamic modeling with finite differences and marker in cell: theory, teaching and examples

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Take-home messages

1. **Numerical geodynamic modeling** is an exciting and rapidly evolving field.

2. **Simplicity and efficiency can (sometimes) win over mathematical beauty and numerical sophistication.**
First paper in 1970

Fig. 5. Temperature regime for a spreading velocity of 1 cm/yr with conductive heat transfer only.

First textbooks in 2010
Geodynamic modeling challenges

- Large deformation of complex materials
- Extremely large variability of both time and space scales
- Non-intuitive natural phenomena
- Fundamentally limited accessibility of data
Large deformation

Large deformation in car industry
http://www.mscsoftware.com/product/dytran

Large deformation in geodynamics
Sandbox experiments

Numerical

I2ELVIS

Univ. Parma

IFP Rueil-Malmaison

Gerya & Yuen (2007)
Geophysical Fluid Dynamics, D-ERDW, ETH–Zurich
Geophysical Fluid Dynamics, D-ERDW, ETH–Zurich
Geophysical Fluid Dynamics, D-ERDW, ETH– Zurich
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Geophysical Fluid Dynamics, D-ERDW, ETH–Zurich
Geophysical Fluid Dynamics, D-ERDW, ETH–Zurich
Geophysical Fluid Dynamics, D-ERDW, ETH– Zurich
Geophysical Fluid Dynamics, D-ERDW, ETH–Zurich
An egg does not look like a chicken. Therefore, seeing 1000 chickens does not help to understand how an egg looked like…
Non intuitive phenomena

past

???

present
Why staggered finite differences with marker in cell (SFD-MIC)?

Because it is a universal flexible approach with potentially unlimited number of applications

- Easy to learn
- Easy to implement
- Easy to adapt for new problems

- Stable convergence
- Low computational costs
- Simple parallelization
Theory
Basic equations (2D example)

Conservation of energy

$$\rho C_p \left( \frac{DT}{Dt} \right) = -\frac{\partial q_x}{\partial x} - \frac{\partial q_z}{\partial z} + H_r + H_a + H_s + H_L,$$

Conservation of mass

$$\frac{D \ln \rho}{Dt} + \frac{\partial v_x}{\partial x} + \frac{\partial v_z}{\partial z} = 0$$

Conservation of momentum

$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xz}}{\partial z} - \frac{\partial P}{\partial x} = -\rho(T, P, c)g_x(x, z, t)$$

$$\frac{\partial \sigma_{zx}}{\partial x} + \frac{\partial \sigma_{zz}}{\partial z} - \frac{\partial P}{\partial z} = -\rho(T, P, c)g_z(x, z, t),$$
Simplest method of numerical solution

Combination of finite-differences, on staggered grid, and the moving marker technique

\[
\frac{\partial P}{\partial x} = \frac{(P_2 - P_1)}{\Delta x}
\]
2D (left) and 3D (right) staggered grid used for discretisation of momentum, continuity, Poisson and temperature equations in the case of visco-elasto-plastic flow with variable viscosity and thermal conductivity

(Gerya, 2010)
**Why staggered grid?**

*It is a natural way of discretizing thermo-mechanical equations with finite differences*

**a)** incompressible continuity equation

\[
\frac{\partial u_x}{\partial x} + \frac{\partial v}{\partial y} = 0
\]

**b)** continuity equation stencil

**c)** discretized form

\[
\left( \frac{v_{x(i-1,j)} - v_{x(i-1,j-1)}}{\Delta x} + \frac{v_{y(i,j-1)} - v_{y(i-1,j-1)}}{\Delta y} \right) = 0
\]

(Gerya, 2010)
Markers-nodes interpolation

**distance-dependent average**

\[ B_{i,j} = \frac{\sum_{m} B_m w_m(i,j)}{\sum_{m} w_m(i,j)} , \]

\[ w_m(i,j) = \left( 1 - \frac{\Delta x_m}{\Delta x} \right) \times \left( 1 - \frac{\Delta y_m}{\Delta y} \right) \]

Fig. 8.8 Stencil of 2D grid used for the interpolation of physical properties from the markers to the nodes. The dashed boundary indicates the area from which markers are used for interpolating properties to node \((i, j)\) in the case of a local interpolation scheme.

\[ B_m = B_{i,j} \left( 1 - \frac{\Delta x_m}{\Delta x} \right) \left( 1 - \frac{\Delta y_m}{\Delta y} \right) + B_{i,j+1} \frac{\Delta x_m}{\Delta x} \left( 1 - \frac{\Delta y_m}{\Delta y} \right) + B_{i+1,j} \left( 1 - \frac{\Delta x_m}{\Delta x} \right) \frac{\Delta y_m}{\Delta y} + B_{i+1,j+1} \frac{\Delta x_m \Delta y_m}{\Delta x \Delta y} , \]

Fig. 8.9 Stencil of a 2D grid used for the interpolation of physical properties from nodes to markers.

(Gerya, 2010)
Why markers?

- Markers are a natural way to *advect and update material properties*
- Markers are not connected to each other but have a group memory

\[ g_x = 10 \text{ m/s} \]

\[ g_x = 10 \text{ m/s} \]

\[ g_x = 0 \text{ m/s} \]
Numerical Algorithm

1. Criterion for elastic time stepping $\Delta t$ for momentum equation
2. Calculation of scalar and tensor properties (density, stress etc.) for markers, interpolation of these properties to nodes
3. Solving continuity and momentum equations by direct method
4. Criterion for time stepping $\Delta t_m$ for material displacement
5. Interpolating of tensor changes from nodes to markers
6. Calculation of shear and adiabatic heating
7. Criterion for time stepping $\Delta t$ for temperature equation
8. Implicit solving of temperature equation by direct method
9. Interpolating of temperature changes from nodes to markers
10. Advection of markers by velocity field calculated at Step 1 and rotating of elastic stress on markers by vorticity field

“non-diffusive” interpolation

(Gerya, 2010)
Adaptive Mesh Refinement (AMR)

Gerya et al. (2013)
Gerya et al. (2013)
Gerya et al. (2013)
Teaching
(from scratch)
Abstract
In this 13-week sequence, students learn how to write programs from scratch to solve partial differential equations that are useful for Earth science applications. Programming will be done in MATLAB and will use the finite-difference method and marker-in-cell technique. The course will emphasize a hands-on learning approach rather than extensive theory.

Objective
The goal of this course is for students to learn how to program numerical applications from scratch. By the end of the course, students should be able to write state-of-the-art MATLAB codes that solve systems of partial-differential equations relevant to Earth and Planetary Science applications using finite-difference method and marker-in-cell technique. Applications include Poisson equation, buoyancy driven variable viscosity flow, heat diffusion and advection, and state-of-the-art thermomechanical code programming. The emphasis will be on commonality, i.e., using a similar approach to solve different applications, and modularity, i.e., re-use of code in different programs. The course will emphasize a hands-on learning approach rather than extensive theory, and will begin with an introduction to programming in MATLAB.
A provisional week-by-week schedule (subject to change) is as follows:

Week 1: Introduction to the finite difference approximation to differential equations. Introduction to programming in Matlab. Solving of 1D Poisson equation.


Week 3: Solving momentum and continuity equations in case of constant viscosity with stream function/vorticity formulation.


Weeks 5: Conservative finite differences for the momentum equation. "Free slip" and "no slip" boundary conditions. Solving momentum and continuity equations in case of variable viscosity using pressure-velocity formulation with staggered grid.


Week 7: Advection in 2-D with Marker-in-cell method. Combining flow calculation and advection for buoyancy driven flow.

Week 8: "Free surface" boundary condition and "sticky air" approach. Free surface stabilization. Runge-Kutta schemes.

Week 9: Solving 2D heat conservation equation in case of constant thermal conductivity with explicit and implicit approaches.

Week 10: Solving 2D heat conservation equation in case of variable thermal conductivity with implicit approach. Temperature advection with markers. Creating thermomechanical code by combining mechanical solution for 2D buoyancy driven flow with heat diffusion and advection based on marker-in-cell approach.

Week 11: Subgrid diffusion of temperature. Implementing subgrid diffusion to the thermomechanical code.

Week 12: Implementation of radioactive, adiabatic and shear heating to the thermomechanical code.

Week 13: Implementation of temperature-, pressure- and strain rate-dependent viscosity, temperature- and pressure-dependent density and temperature-dependent thermal conductivity to the thermomechanical code. Final project description.

GRADING will be based on weekly programming homeworks (50%) and a term project (50%) to develop an application of their choice to a more advanced level.

Literature

Taras Gerya, Introduction to Numerical Geodynamic Modelling, Cambridge University Press 2010
Examples

(many are nature-inspired)
Melt intrusion into the crust
Volcanism refers to spectacular magma eruptions that fascinate the general public but the less flamboyant effects of underground magma expansion, called plutonism, remain captivating to earth scientists. Since James Hutton conceived the idea of plutonism in the late 18th century (e.g., Ellenberger, 1994) the formation of large magma bodies, the plutons, eludes full understanding. Research on the topic has, however, been much focused on the emplacement...
Melts crossing the lithosphere...
neutral buoyancy level

cold and strong lower crust
neutral buoyancy level
neutral buoyancy level
neutral buoyancy level
neutral buoyancy level
neutral buoyancy level
neutral buoyancy level
neutral buoyancy level
neutral buoyancy level
Why does heavy intrusion go up in the lower density crust?!
Deep roots of the intrusion stabilise it above the neutral buoyancy level.
We employ a visco-elasto-plastic rheology with experimentally calibrated flow laws and elastic shear moduli computed from stable phase assemblages for each lithology (8). The plastic strength is taken to be dependent on pore fluid pressure $P_{\text{fluid}}$ such that (13):

$$\sigma_{\text{yield}} = \cos(\varphi)C + \sin(\varphi)P$$

Plastic strength of the crust decreases with decreasing depth (pressure)

where $C$ is cohesion (residual strength at $P=0$), $\varphi$ is effective internal friction angle ($\varphi_{\text{dry}}$ stands for dry rocks) and $\lambda = \frac{P_{\text{fluid}}}{P_{\text{solid}}}$ is the pore fluid pressure factor, $P_{\text{solid}} = P$ corresponds to mean stress on solids.
neutral buoyancy level

warm and weak lower crust

Weak lower crust
neutral buoyancy level

Weak lower crust
neutral buoyancy level

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Weak lower crust
Variations in intrusion morphology

Gerya & Burg (2007)
Surface evolution of Venus

Venus: visible-light
Venus surface: 475°C, no liquid water
64 Nova structures
Becuma Mons nova

(Krassilnikov and Head, 2003)
512 Corona structures

(a) Aramalti Corona [25.5°S, 82.0°E], a concentric corona ~350 km in diameter which displays a well-defined annulus of concentric fractures. Note the small-scale volcanism in the centre and larger-scale volcanism where radar-dark material has flooded the topographic moat.

(b) Aruru Corona [9.0°N, 262.0°E], has a diameter of ~450 km and shows evidence of extensive interior and exterior volcanism.

(Grindrod and Hoogenboom, 2006)
Plume-crust interactions

(Krassilnikov and Head, 2003)

(Dombard et al., 2007)
3D high-resolution thermo-mechanical model
Stage 2

 nova rise

1.2 Myr

log viscosity (Pa s)

-200 0 200 400 600

topography (m)

18 20 22 24

100 150 200 250 300

km

concentric fractures

stellate fractures

radial fractures

solid crust

partially molten crust

incipient convection cell

solid magma

incipient plume

crust

magma

plume

solid

molten

viscosity

temperature

incipient convection cell

N

B

B'

A

A'
Stage 5

- Topography (m)
- Log viscosity (Pa s)

Subsiding corona
- Central rise
- Crustal wedge
- Trench
- Outer rise
- Circular depression

8.9 Myr

Log viscosity (Pa s) - Temperature (K)
- Solid molten crust
- Magma
- Plume

Spreading corona
- Convection cell

Viscosity
- Temperature

Cooling mantle plume
Radial model topography (Smrekar and Stofan, 1997)

Topographic groups of coronae:
- central depression
- stellate fractures
- topography rise

Numerical Model

Becuma Mons Nova

50 km
Initiation of plate tectonics

Global picture

(http://www.odsn.de/odsn/services/paleomap/animation.html)
How did plate tectonics start?

Pre-plate tectonics Earth
>3 billion years ago

Modern Earth
How does subduction initiate under present-day conditions?

**INDUCED**
- Transference
- Polarity Reversal

**SPONTANEOUS**
- Passive Margin Collapse
- Transform Collapse

- S = Suture
- = Subducting Plate
- T = Transform Fault or Fracture Zone

Mussau Trench
Miocene Solomon Arc
No Cenozoic Examples
Eocene Western Pacific
Indian Ocean (someday?)

Stern (2004)

Most present-day subduction initiation mechanisms require acting plate forces and/or pre-existing zones of lithospheric weakness, which are themselves consequences of plate tectonics.
Plume-induced subduction initiation

Ueda et al. (2008)
(1) oceanic plateau formation by plume-induced magmatism

Gerya et al. (Nature, 2015)
(2) formation of an incipient trench and a descending nearly-circular slab at the plateau margins

Gerya et al. (Nature, 2015)
(3) tearing of the circular slab under its own weight
(4) formation of several self-sustained retreating subduction zones

Gerya et al. (Nature, 2015)
(5) cooling of the new plate, initiation of spreading centers and transform boundaries within this plate

Gerya et al. (Nature, 2015)
(5) cooling of the new plate, initiation of spreading centers and transform boundaries within this plate

Gerya et al. (Nature, 2015)
If you want to imagine how plate tectonic started...

Scientists think that a mantle plume, like the one that created a vast basalt deposit that underlies much of the Caribbean Sea, might have triggered subduction and kick-started global plate tectonics.

How the shell of ancient Earth cracked, giving rise to moving continents

By Julia Rosen | Nov. 11, 2015, 5:30 PM
Caribbean-like structure can form spontaneously.

bsayna1100.pm topo z = 405  time = 12.6948 Myr

500 km
Not exclusive to Earth …

Artemis corona

1000 km
Oceanic transform faults: how and why do they form?
Popular view on transforms: inheritance concept

Lister et al. (1986)
Inheritance concept

- Continent
- Preexisting structures
- Continent
- Rifting
- Continent
- Spreading
- Continent
- Ocean
Inheritance concept

Two transform faults

Two bents on the margin

Two transform faults

500 km
Continental rifting: no clear transform precursors

Bothworth (1986)
This is how faults should be oriented in extension

Chemenda et al. (2002)
freezing wax experiments

Oldenburg and Brune (1972)

Variable-speed fan

Tray for wax (5 by 30.5 by 45 cm)

Orthogonal ridge transform pattern

Movable stick
freezing wax experiments

Oldenburrug and Brune (1972)
Transform faults can be emergent!

Fig. 5. Two possible modes for adjustment of a ridge to a change in spreading direction. **A**, The ridge readjusts as a unit taking on a new direction by time \( t_2 \) after \( 3N \) km of spreading has occurred. **B**, The ridge breaks into segments, each piece becoming realigned by time \( t_1 \) after \( N \) km of spreading.
Spontaneously emerging transforms:

how is this possible?
topography, km

viscosity, Pa s

Gerya (Science, 2010)
Gerya (Science, 2010)
Gerya (Science, 2010)
A

B

C

D

Gerya (Science, 2010)
Gerya (Science, 2010)
Gerya (Science, 2010)
topography, km

viscosity, Pa s

$\nu_x$, m/s

Gerya (Science, 2010)
topography, km

viscosity, Pa s

Gerya (Science, 2010)
Model without gravity

Model with doubling of spreading rate

Gerya (Science, 2010)
How do inherited transform faults form?
0.4 Myr

Bathymetry (km)

Log viscosity (Pa s)

incipient spreading centers

rift tip

accommodation zone

rift tip

rift tip

accommodation zone
0.5 Myr

Bathymetry (km)

Log viscosity (Pa s)

propagating spreading centers

accommodation zone

accommodation zone
1.2 Myr

Bathymetry (km)

Log viscosity (Pa s)

- growing spreading centers
- rotating transform fault
- rotating transform fault
2.1 Myr

Bathymetry (km)

Log viscosity (Pa s)

growing oceanic crust
young transform fault
ancient rift tip
young transform fault
3.3 Myr

Bathymetry (km)

Log viscosity (Pa s)

growing inactive fracture zones
transform fault
Transform fault starts as **plate-fragmentation** structure and evolve into **plate-growth** structure: the difference is as in between broken glass and snowflake.
Continental breakup induced by a mantle plume
Continental breakup induced by a mantle plume

Burov and Gerya (Nature, 2014)
Stressed Plate + No Plume vs. Plume + Non-stressed Plate

Burov and Gerya (Nature, 2014)
Balloon = Stressed Plate
Pin = Plume
Stressed Plate with a Craton + Plume

Koptev et al. (Nature Geoscience, 2015)
Extending geodynamic models for self-gravitation: spherical Cartesian approach

Poisson equation (self-gravitation)

\[ \frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial z^2} = 4K\pi\gamma\rho(P, T, c) \]
Self-gravitation (spherical Cartesian approach)

(Gerya et. Al., 2013)
Self-gravitation (spherical Cartesian approach)

silicate
iron
silicate
MODEL 4
MODEL 4
MODEL 4

pibc28. 28 0.5031 Myr
MODEL 4
MODEL 4

pibc43. 43 0.5045 Myr
MODEL 4
MODEL 4
MODEL 4
MODEL 4
Extending geodynamic models for seismicity

1. Slow tectonic loading
2. Rate-dependent friction
3. Visco-elastic stress relaxation
4. Self-consistent faults
5. Seismo-thermo-mechanical coupling
Modified “geodynamic” equations

Conservation of momentum (with inertia)

\[
\frac{\partial \sigma'_{xx}}{\partial x} + \frac{\partial \sigma'_{xy}}{\partial y} - \frac{\partial P}{\partial x} = \rho \frac{Dv_x}{Dt}
\]

\[
\frac{\partial \sigma'_{yx}}{\partial x} + \frac{\partial \sigma'_{yy}}{\partial y} - \frac{\partial P}{\partial y} = \rho \frac{Dv_y}{Dt} - \rho g
\]

Plastic rheology (with rate-dependent friction)

\[
\sigma_{yield} = C + \mu_{eff} \cdot P
\]

\[
\mu_{eff} = \mu_s (1 - \gamma) + \mu_s \frac{\gamma}{1 + V/V_c}
\]
Seismo-thermo-mechanical modeling (STM)

Paper 1: Corbi et al. (2013)

Paper 2: van Dinther et al. (2013)
STM: proof of a concept

van Dinther et al. (2013)
van Dinther et al. (2013)
STM: proof of a concept

van Dinther et al. (2013)
STM: application to nature

Herrendörfer et al. (Nature Geoscience, 2013)
STM: application to nature

Herrendörfer et al. (Nature Geoscience, 2013)
STM: application to nature

Interseismic phase

Coseismic phase

Van Dinther et al. (2013)
STM: application to nature

Megathrust events

Van Dinther et al. (2013)
STM: application to nature

Van Dinther et al. (2013)
STM: application to nature

Dal Zilio et al. (submitted)
STM: application to nature

Guttenberg-Richter law

Dal Zilio et al. (submitted)
STM: application to nature

**Guttenberg-Richter law**

- **Graph (a)**
  - Number of earthquakes vs. magnitude (Mw)
  - Data points for different convergence rates (1 cm/yr, 3 cm/yr, 5 cm/yr)
  - B-values: 1.25, 1.10, 0.97

- **Graph (b)**
  - Relationship between b-value and convergence rate
  - Linear regression: $y = -0.07x + 1.31$

- **Graph (c)**
  - Relationship between b-value and shear stress (MPa)
  - Linear regression: $y = -0.0024x + 1.6362$

**Dal Zilio et al. (submitted)**
Meteorite impacts

*Inertia is treated with markers*
Markers, $t = 0.17781 \text{ s.}$
The End (not really...)
Inertia is treated with markers
Marker in cell model

(a) Resolution 71x71

(b) Resolution 101x101

(c) Resolution 151x151

Experiment

Industrial model


Preece and Berg (2004)
Inertia is treated with markers
Markers, $t = 0.15659\, s.$
Markers, t = 0.35393 s.
Extending geodynamic models for hydro-mechanical coupling

Melt bands (Holzman et al., 2005)
Governing equations for (de)compacting visco-plastic incompressible solid and incompressible fluid

(Dymkova and Gerya, 2013)

Matrix deformation and melt migration are treated with markers

Total momentum conservation (in the solid velocity frame)

\[ \frac{\partial\sigma'_{ij}}{\partial x_j} - \frac{\partial p_t}{\partial x_i} = -g_i\rho_t, \]

Mass conservation of the solid

\[ \text{div}(\nu^S) = -\frac{\rho_t - \rho_f}{\eta_{bulk}} \]

Fluid momentum conservation (Darcy)

\[ \nu^D_i = \frac{K}{\eta_f} \cdot \left( \rho_f g_i - \frac{\partial p_f}{\partial x_i} \right) \]

Mass conservation of the fluid

\[ \text{div}(\nu^D) = \frac{\rho_t - \rho_f}{\eta_{bulk}} \]

Matrix porosity evolution

\[ \frac{D\ln(1 - \varphi)}{Dt} = \frac{\rho_t - \rho_f}{\eta_{bulk}} \]

Brittle/plastic deformation (and grains friction) of the solid

\[ \sigma_{\text{yield}} = C + \gamma(p_t - p_f) \]

\( \gamma = 0 - 0.85 \) for \( p_t > p_f \) (confined fractures)

\( \gamma = 1 \) for \( p_t < p_f \) (tensile fractures)
Numerical Example

Melt bands (Holzman et al., 2005)

Model (Gerya et al., Nature 2015)

$V_{x(\text{matrix})}$ (m/s)

fluid fraction

$\log_{10}(\eta)$ (Pa s)

$\log_{10}(\dot{\varepsilon}_{||})$ (1/s)

$\sigma_{||}$ (MPa)

$log_{10}(\text{dissipation})$ (W/m$^3$)

$\lambda_{\text{melt}} = 1 - \frac{p_f}{p_t} \times 10^{-3}$

Melt bands (Holzman et al., 2003)
Staggered finite differences with marker in cell (SFD-MIC)

**SFD-MIC is a universal flexible approach with potentially unlimited number of applications**

Find out what to model

and SFD+MIC will do the job