Computational Geodynamic Modelling I: Spatial Discretisations

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UC San Diego | SCRIPPS INSTITUTION OF OCEANOGRAPHY | IGPP

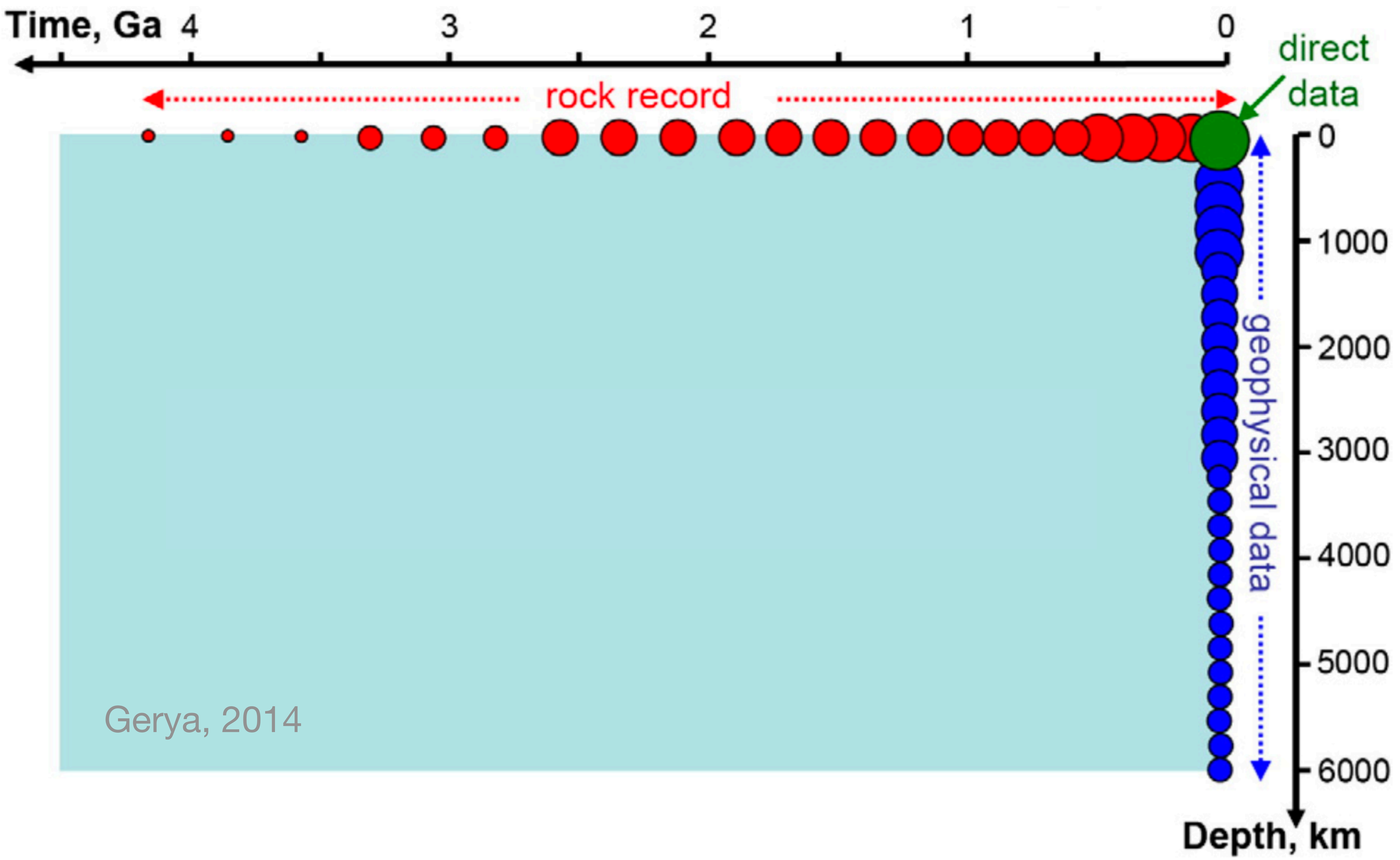
Outline

- **Lecture 1**
  - How we conduct computational geodynamic modelling
- **Lecture 2**
  - Practical challenges in computational geodynamic modelling
- **Lecture 3**
  - How we know our geodynamics models are “correct”

Lecture 1 Outline

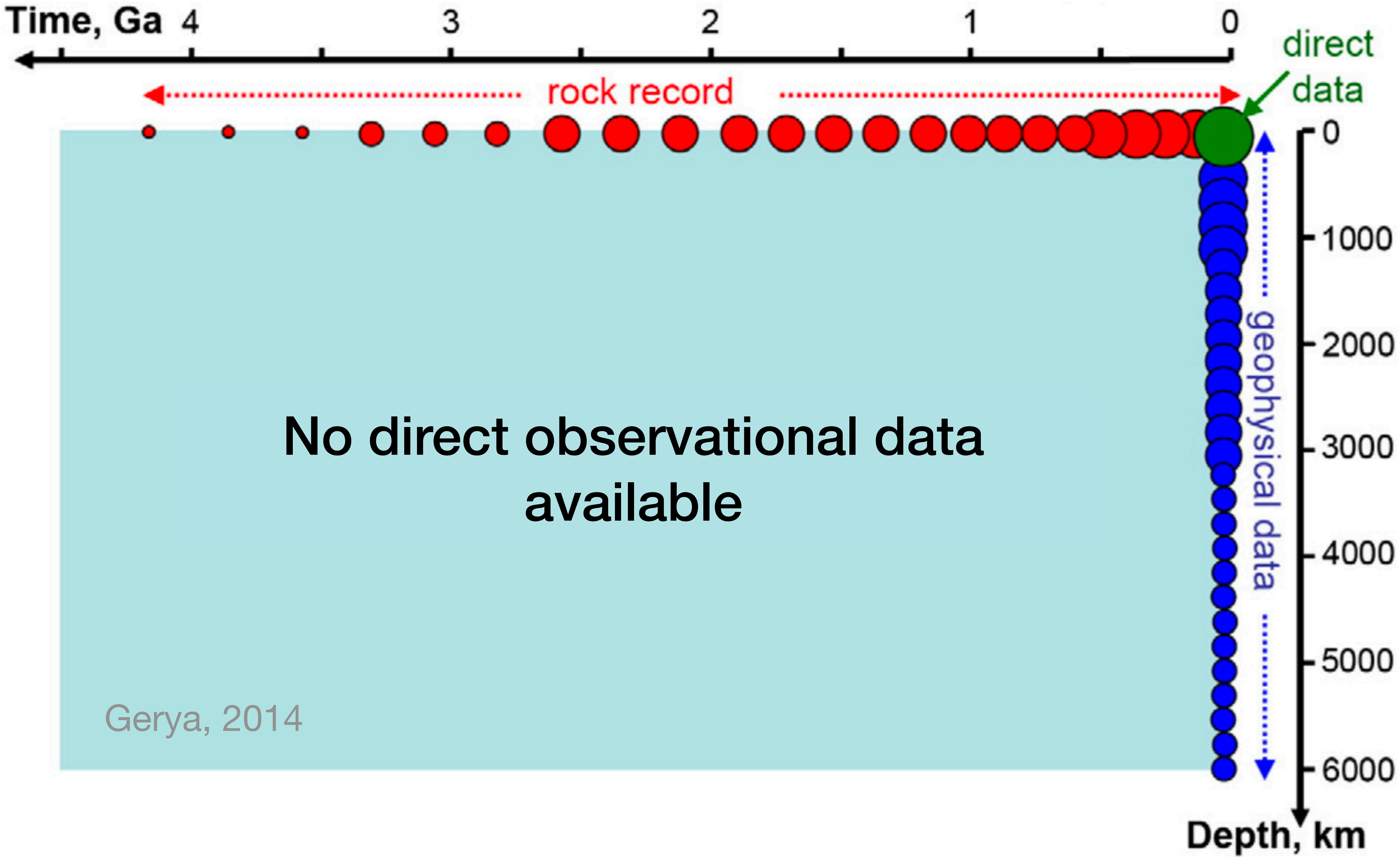
- Why we need geodynamic modelling
- What we model
- How we conduct computational geodynamic modelling
  - Commonly used techniques
- Open source geodynamic modelling tools

Locality of observational constraints

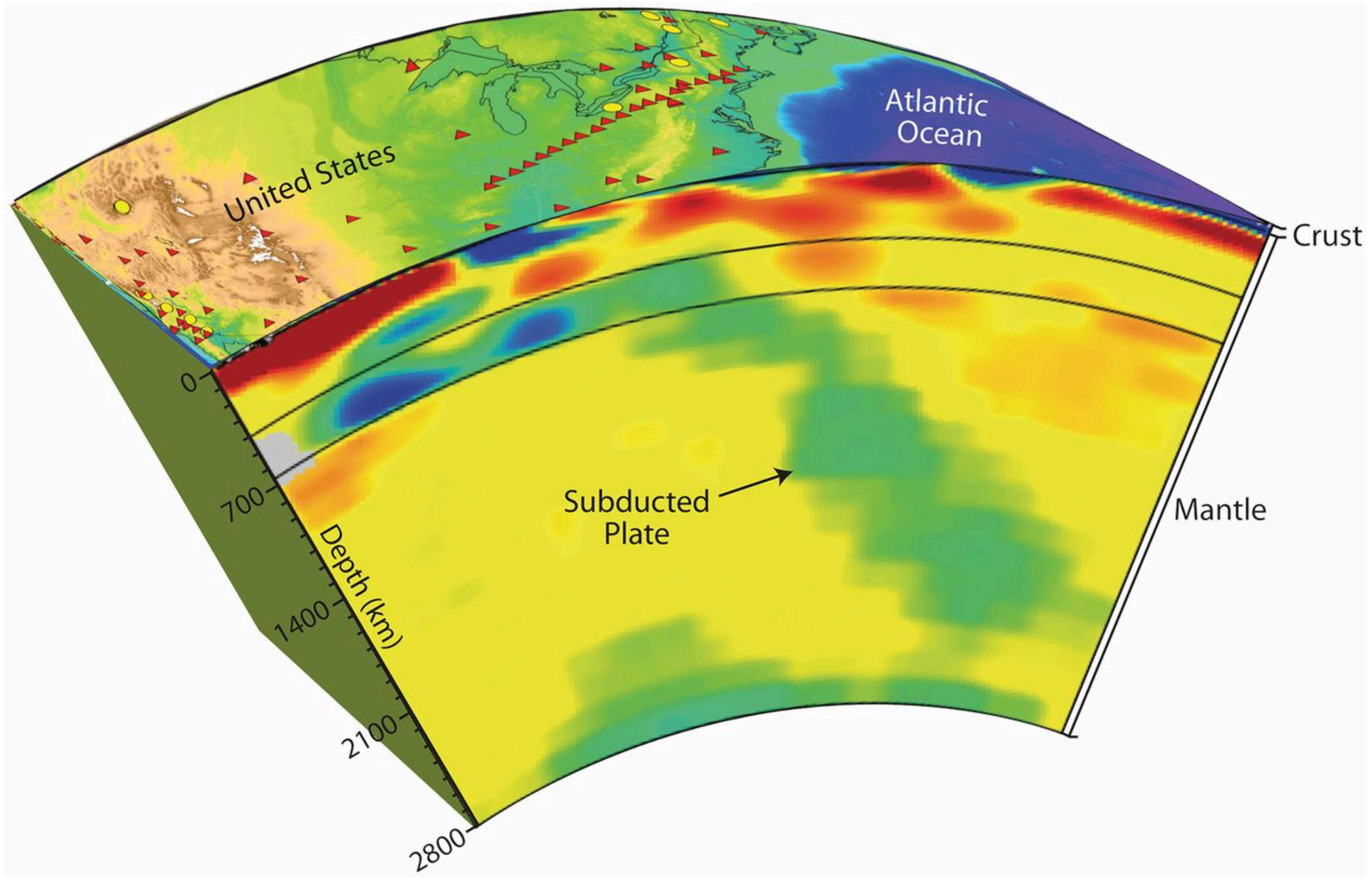


Gerya, 2014

Geology



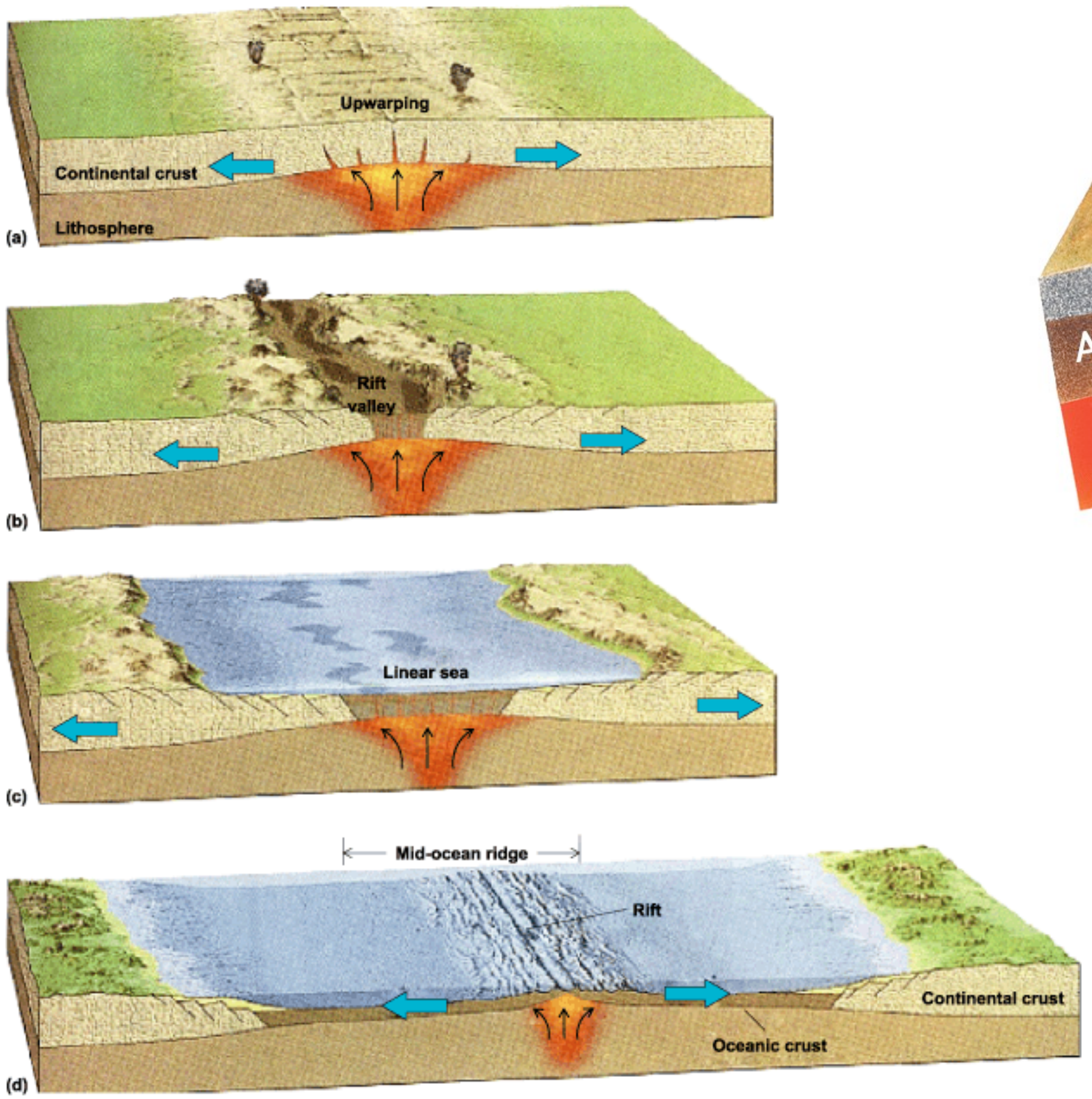
Geophysics

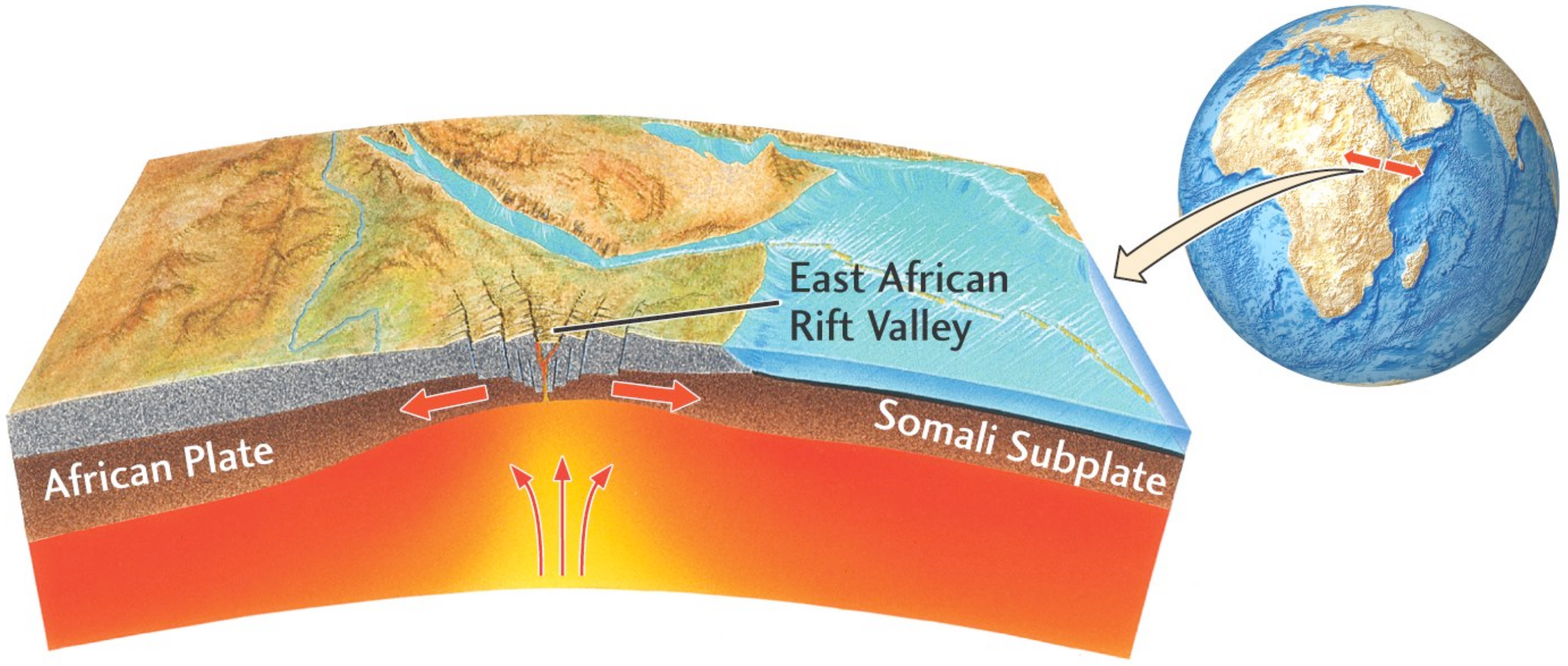


https://www.pnas.org/doi/10.1073/pnas.1909777116

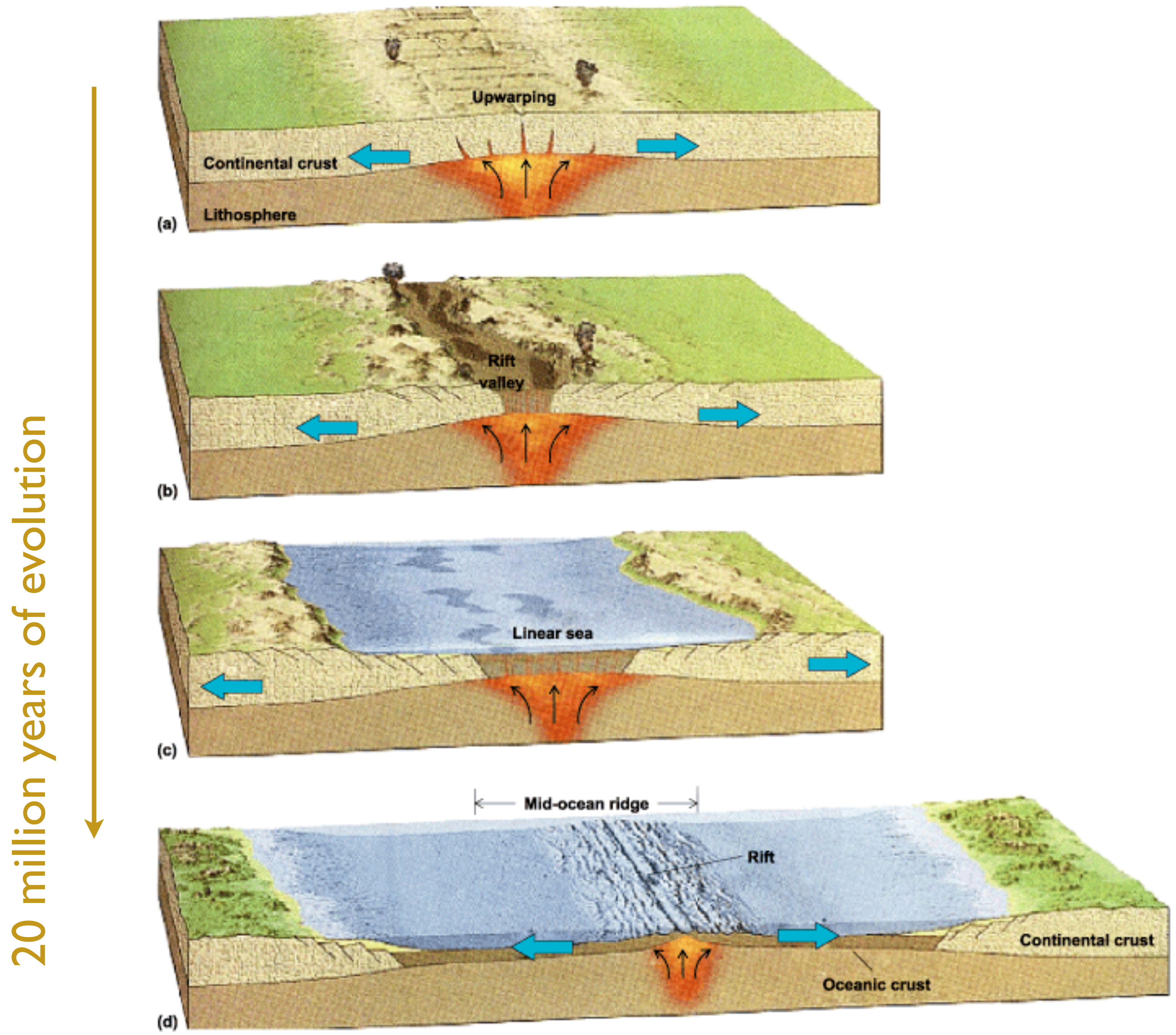
Model motivation

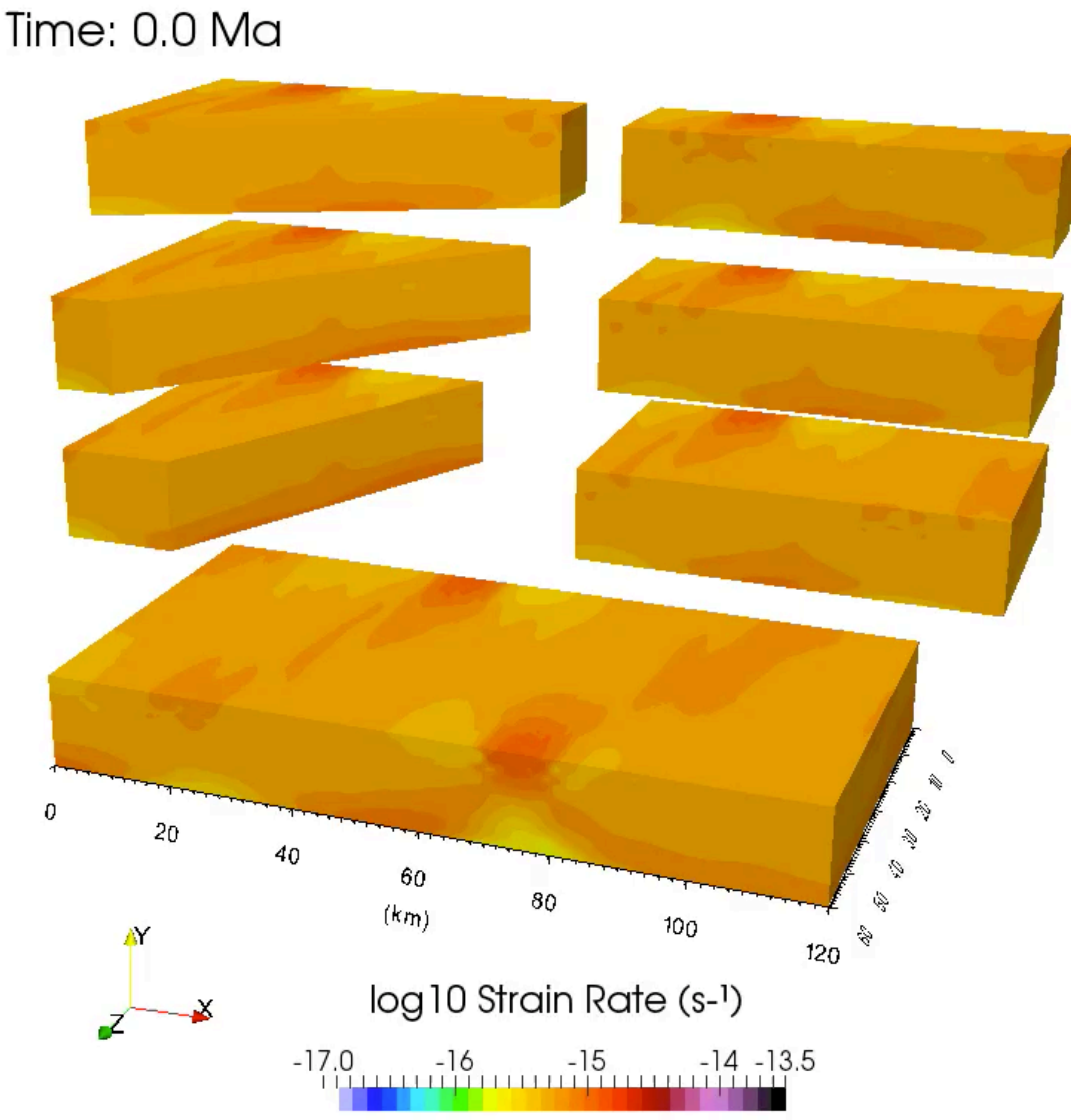
20 million years of evolution





Model motivation





Courtesy of Laetitia Le Pourhiet (UPMC)

Ingredients of a physical model

- A mathematical idealization of the natural world
- Based on physics —> i.e. conservation laws (mass, momentum, energy, …)
- Simplified representation of the complex world is easier to understand
- Requires assumptions
- Capable of describing existing experimental measurements, observations or other empirical data
- Capable of predicting new experimental measurements, observations or other empirical data

Two classes of solutions to physical models

- Analytical
  - Exact solution to the physical model
  - Possibly do not require the use of a computer (i.e. only pen-and-paper)

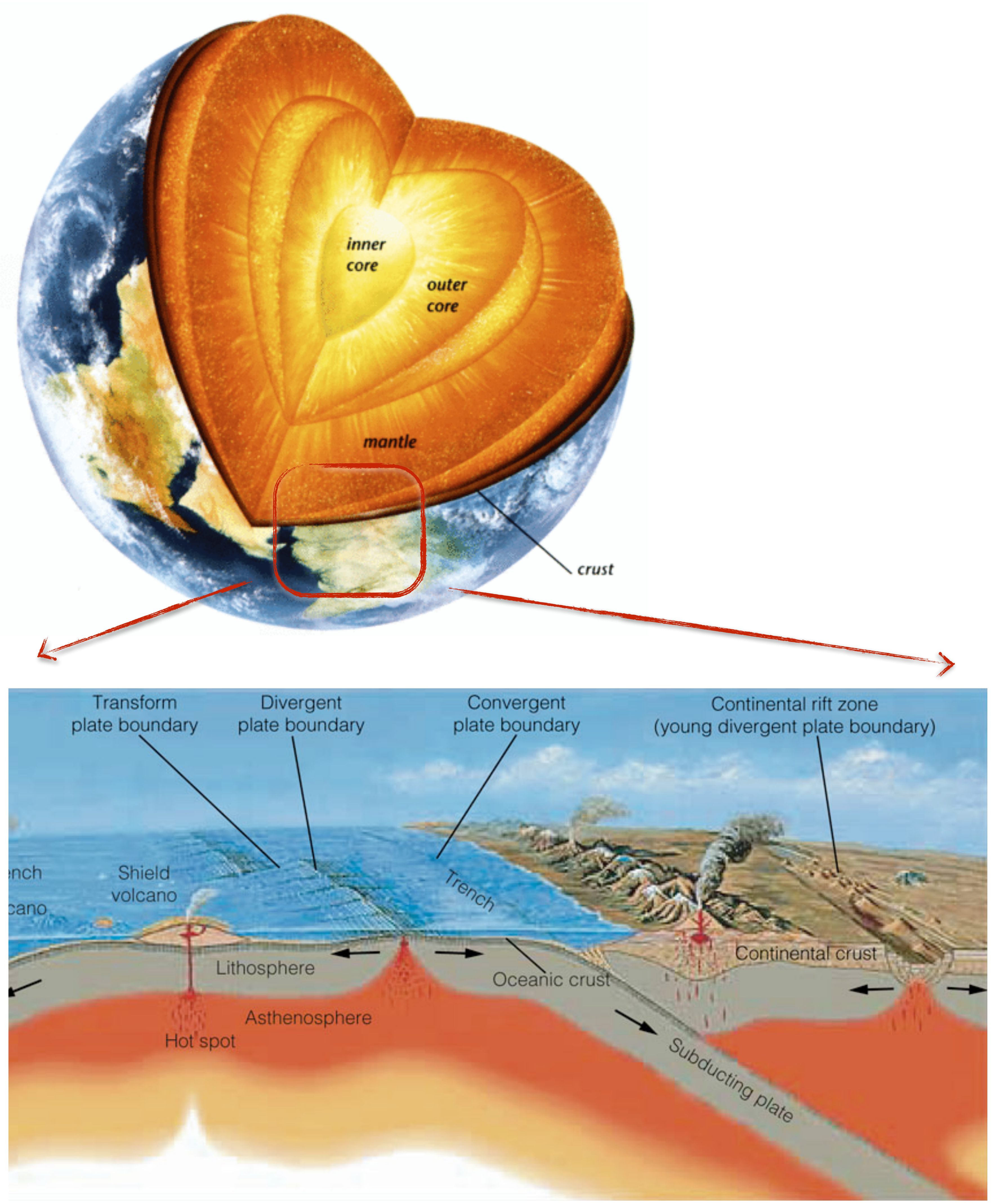
- Numerical
  - Approximate solutions to the physical model
  - Will almost definitely require the use of a computer

Some reasons not to rely on pen-and-paper solutions

- The simplified (minimum complexity) model may not have an analytic solution
  - Dimensionality of the spatial domain
  - Non homogenous material properties
  - Non-linearity
  - Type of boundary conditions

Long time evolution as viscous flow

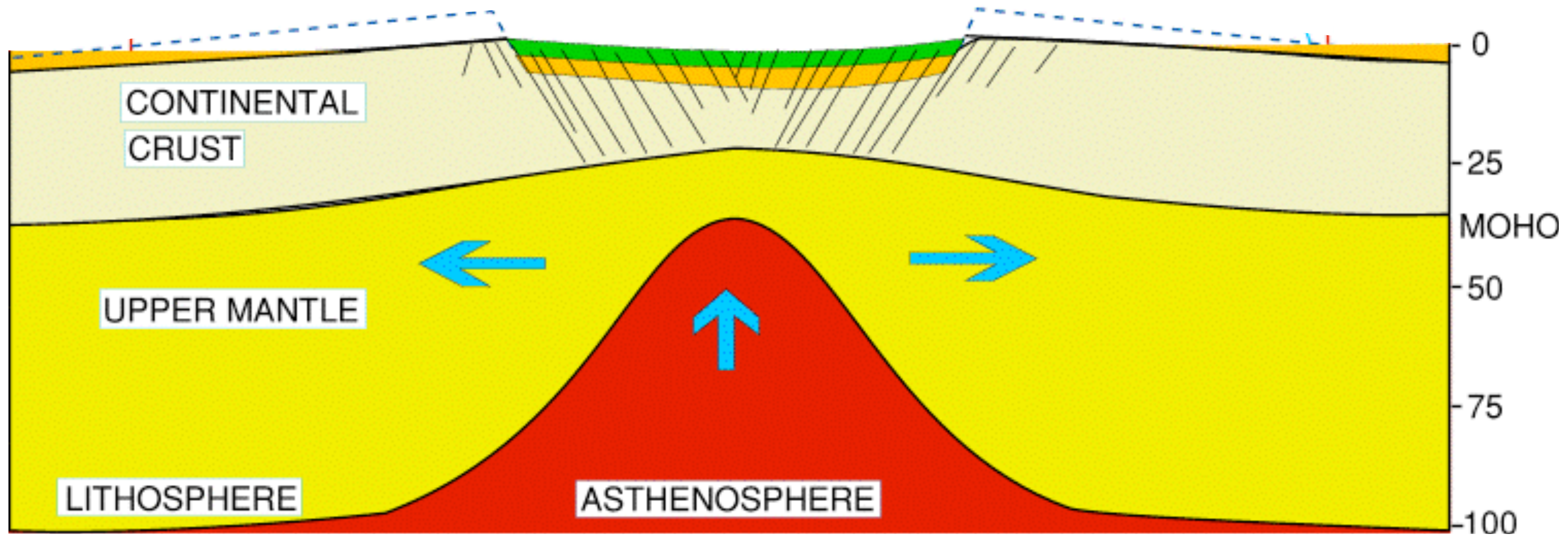
http://asapscience.tumblr.com/post/50419005208/the-earths-center-is-out-of-sync-we-all-know



http://www.korearth.net/lecture/gen_geo/earth_present/ch03/PlateBoundaries.jpg

- Over million year time scales, we assume the following about the mantle-lithosphere-crust system:
  - inertial forces are zero
  - material behaves as a fluid
  - flow driven by buoyancy variations and or imposed velocities

Geodynamic model problem



http://www.le.ac.uk/gl/art/gl209/lecture3

- Conservation of momentum and mass

velocity pressure

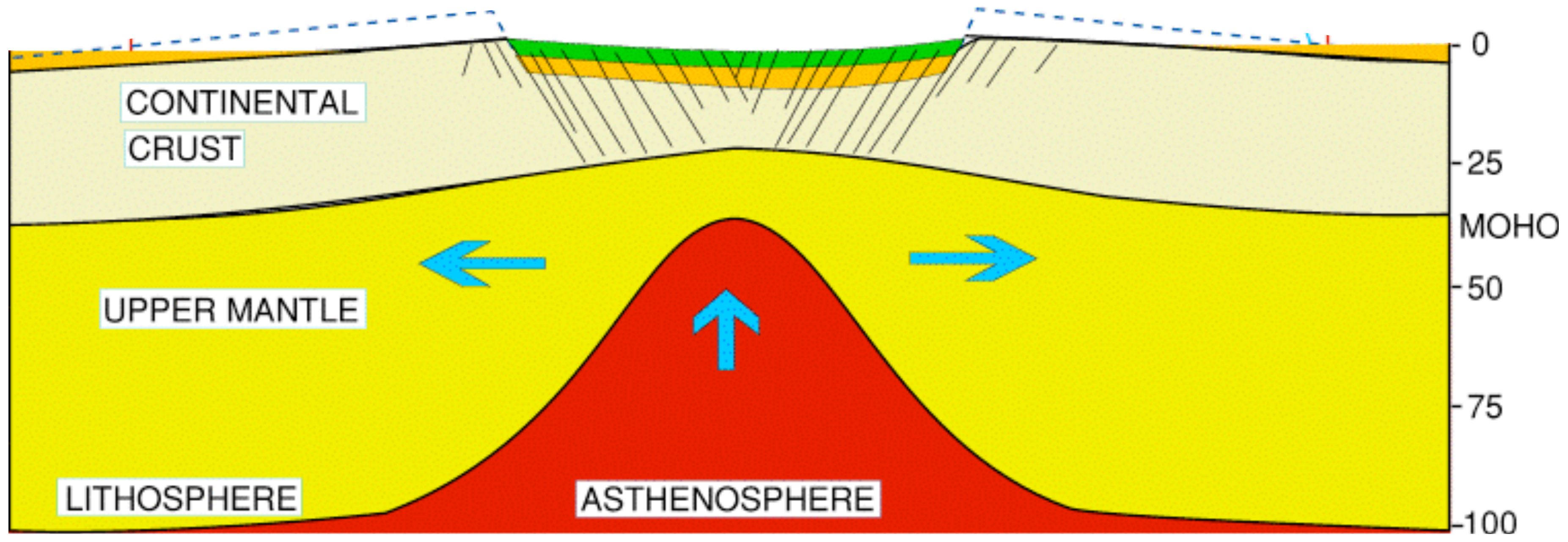
$$\nabla \cdot (\eta(\nabla u + \nabla u^T)) - \nabla p = f$$

$$\nabla \cdot u = 0$$

shear viscosity

volumetric body force

Geodynamic model problem



http://www.le.ac.uk/gl/art/gl209/lecture3

- Conservation of energy

temperature

$$\rho C_p \frac{DT}{Dt} = \nabla \cdot (k \nabla T) + Q$$

density

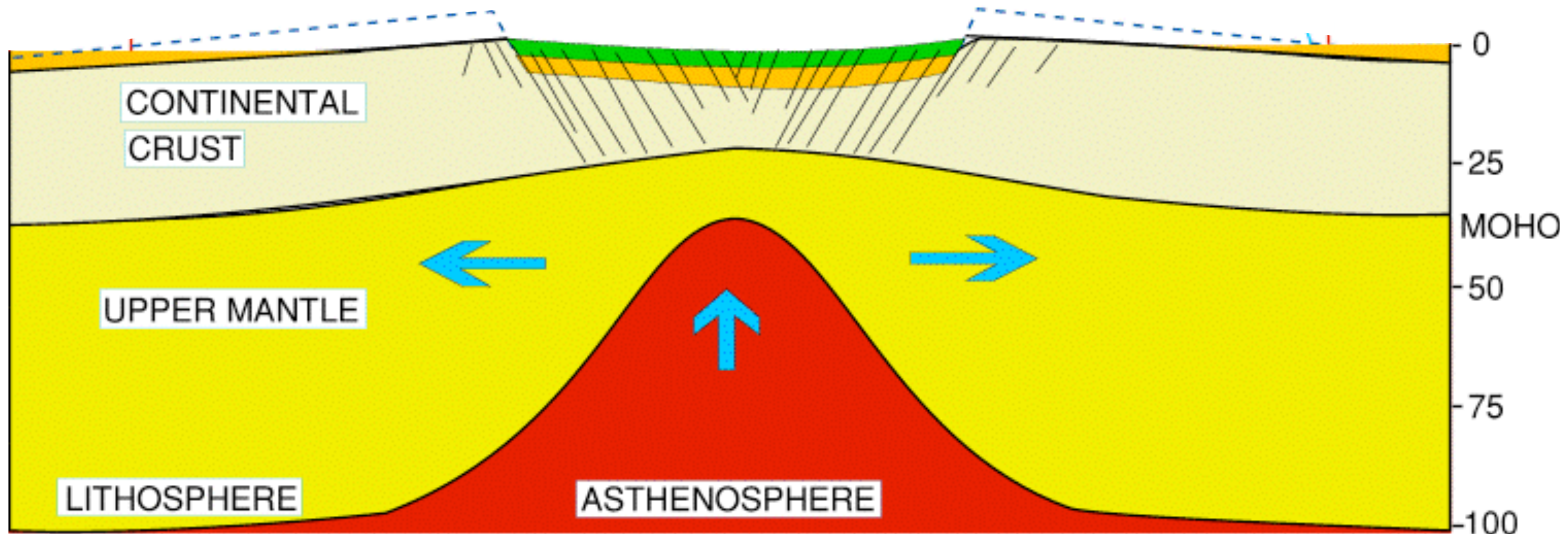
heat capacity

time

thermal conductivity

volumetric heat production

Geodynamic model problem



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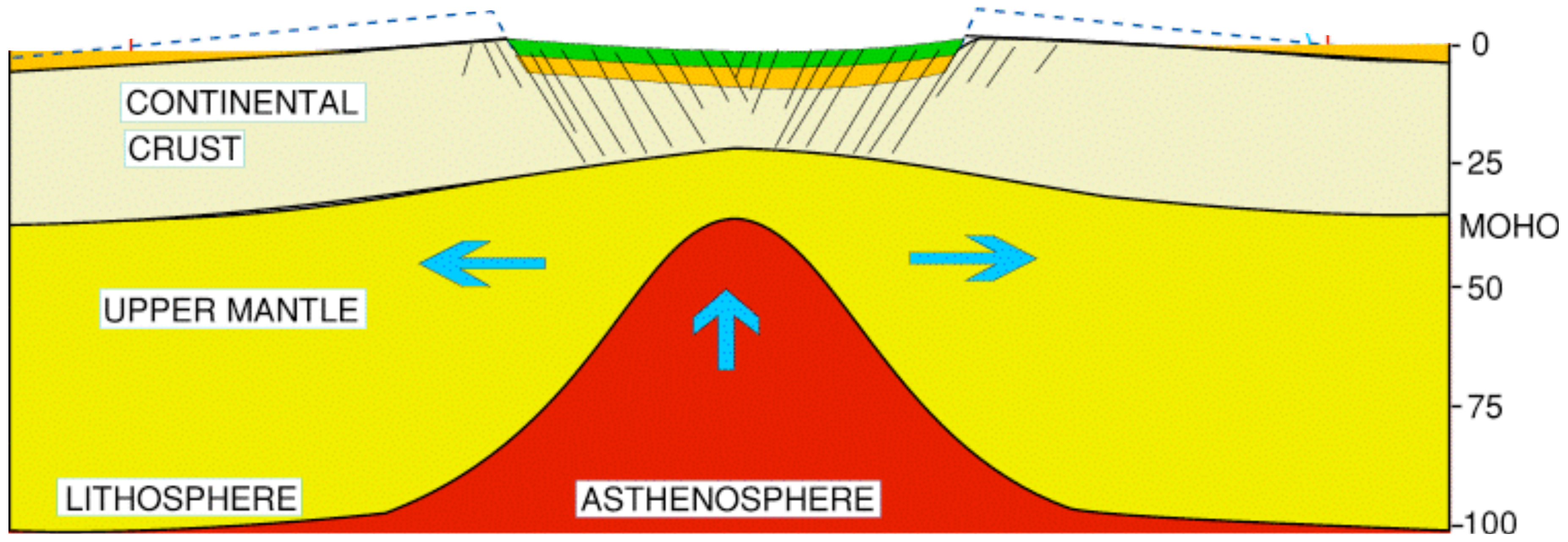
- Coefficient evolution

composition / "rock type"

$$\frac{d\psi}{dt} + \boldsymbol{u} \cdot \nabla\psi = 0$$

velocity

Geodynamic model problem



http://www.le.ac.uk/gl/art/gl209/lecture3

- Conservation of momentum and mass

$$\nabla \cdot \left(\eta(\nabla u + \nabla u^T)\right) - \nabla p = f$$
$$\nabla \cdot u = 0$$

- Conservation of energy

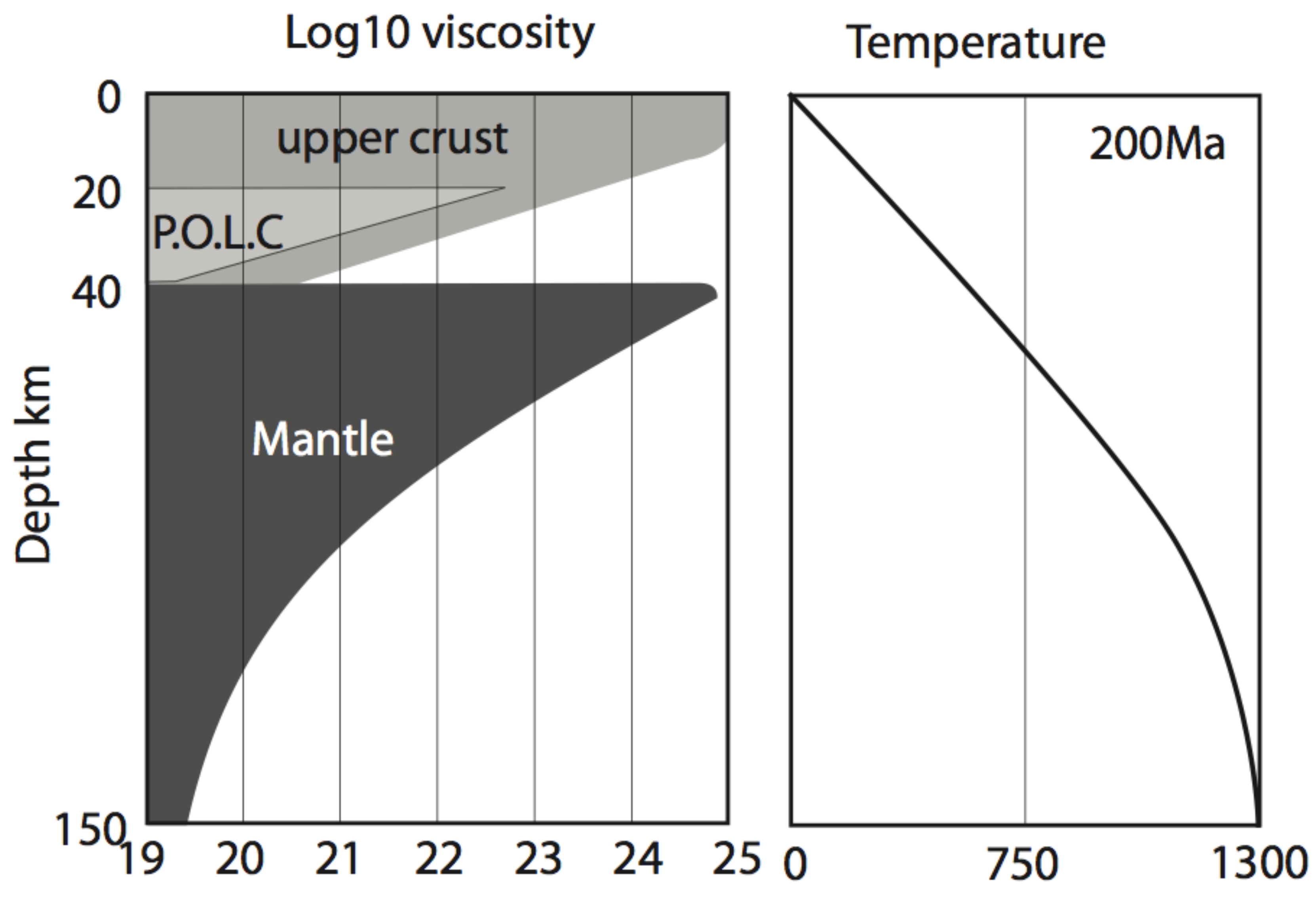
$$\rho C_p \frac{DT}{Dt} = \nabla \cdot (k \nabla T) + Q$$

- Coefficient evolution

$$\frac{d\psi}{dt} + \boldsymbol{u} \cdot \nabla \psi = 0$$

Constitutive behaviour of rocks

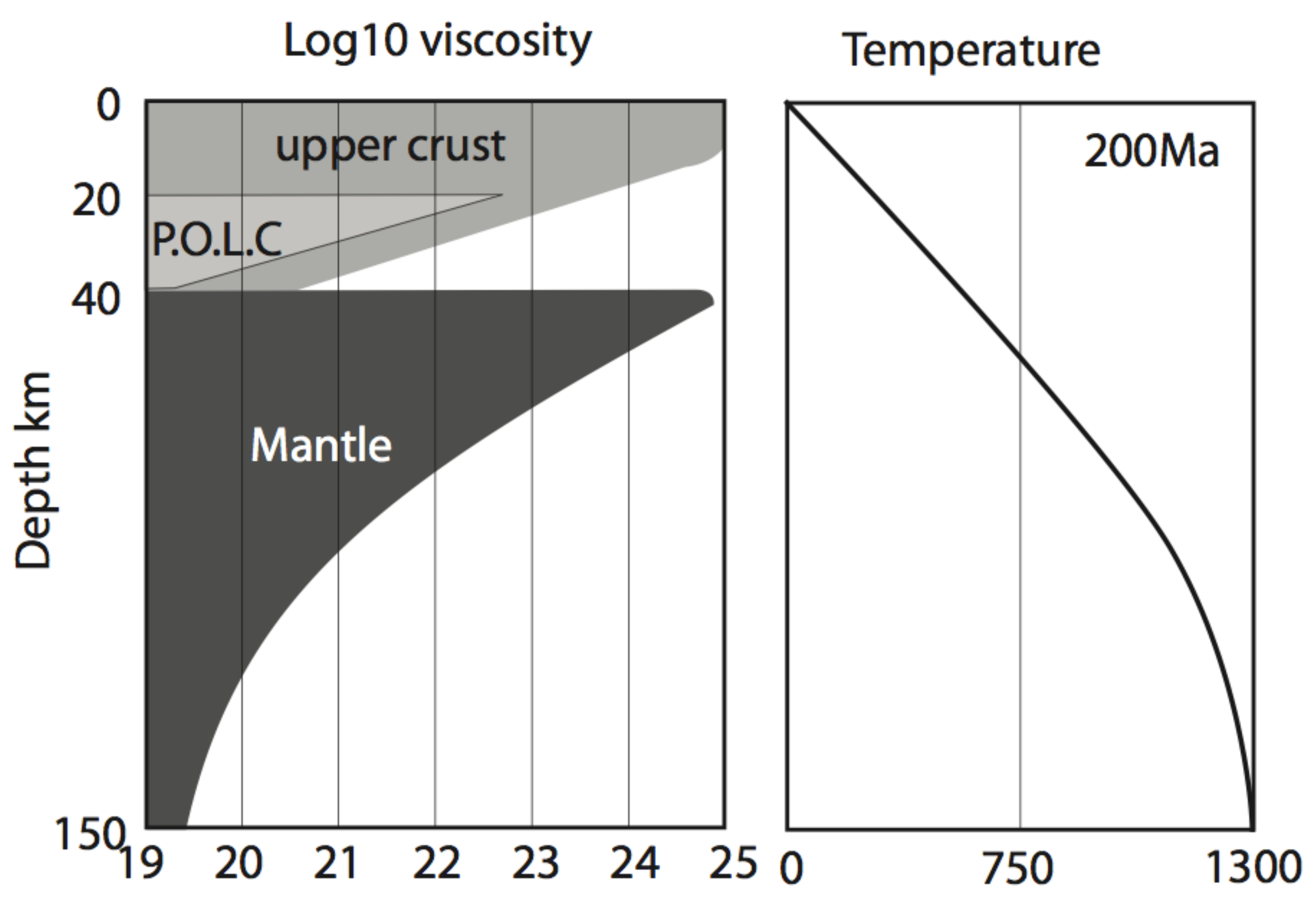
- To first order, temperature controls the viscosity of rocks
- Hot rocks (deep) behave in a ductile fashion
- Cool rocks (shallow) behave in a “brittle” manner
- Constitutive relationships (power-law, visco-plastic)



Constitutive behaviour of rocks

- To first order, temperature controls the viscosity of rocks

- Brittle-ductile behaviour



$$\boldsymbol{\tau} = 2\eta \boldsymbol{D}, \qquad \boldsymbol{D} = \tfrac{1}{2}\left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T\right)$$

$$\eta = A(\sqrt{I_2'})^{\alpha} \exp\left(\frac{E + Vp}{nRT}\right) \qquad I_2' = \tfrac{1}{2} D_{ij} D_{ij}$$

$$F_s := \sqrt{J_2'} - \tau_{\text{yield}}, \qquad \text{where } \tau_{\text{yield}} := C_0 \cos(\phi) + p \sin(\phi), \qquad J_2' = \tfrac{1}{2} \tau_{ij} \tau_{ij}$$

$$\eta = \frac{\tau_{\text{yield}}}{2\sqrt{I_2'}} \qquad \text{if } \sqrt{J_2'} > \tau_{\text{yield}},$$

<— effective non-linear viscosity

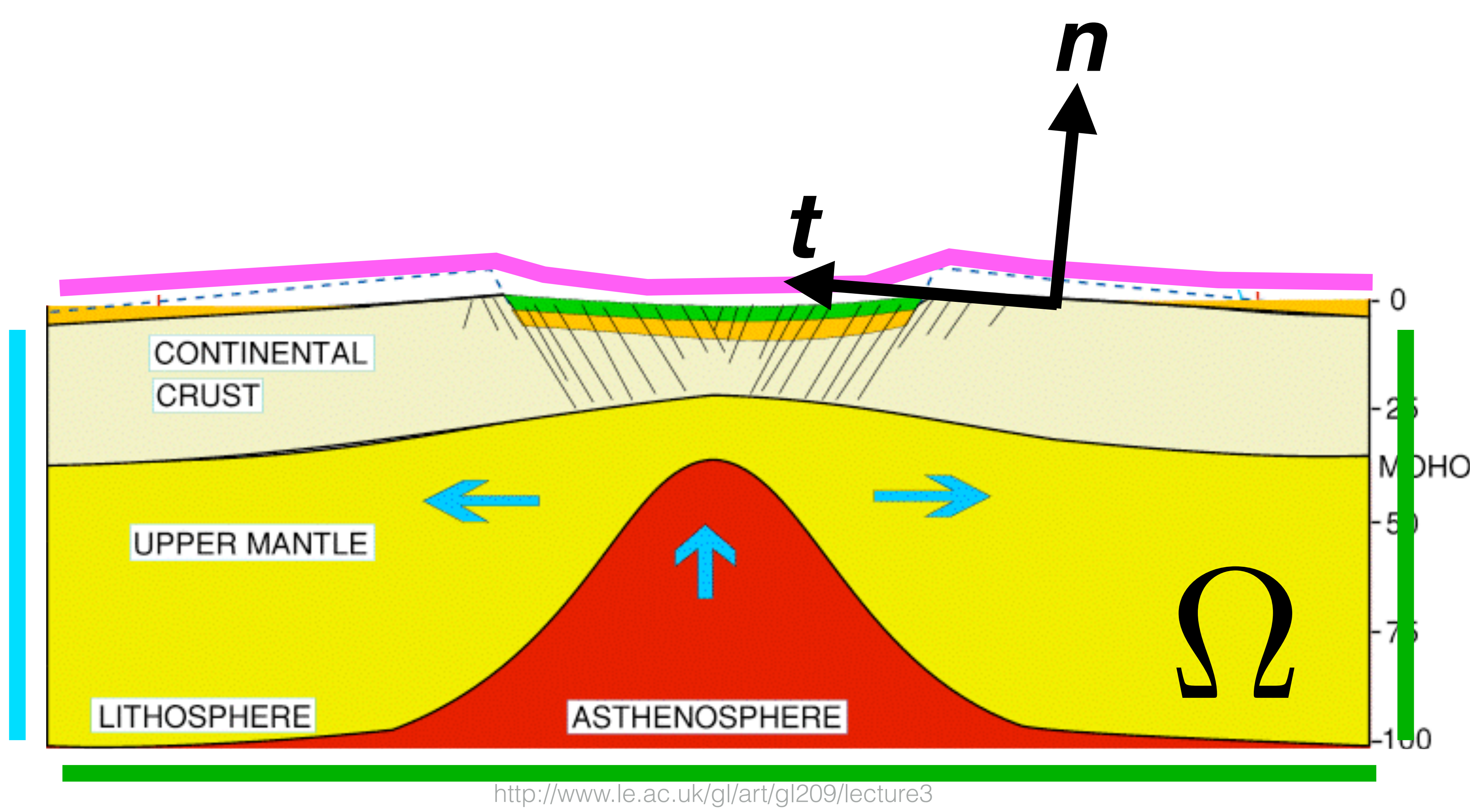
Boundary conditions

$$\boldsymbol{\tau} = 2\eta \boldsymbol{D}, \qquad \boldsymbol{D} = \tfrac{1}{2}\left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T\right), \qquad \boldsymbol{\sigma} = \boldsymbol{\tau} - p\boldsymbol{I}$$

$$\boldsymbol{u} = \boldsymbol{u}_D$$ Dirichlet

$$\boldsymbol{u} \cdot \boldsymbol{n} = u_N, \quad \boldsymbol{t}_k \cdot \boldsymbol{\tau} \cdot \boldsymbol{n} = 0$$ “free slip”

$$\boldsymbol{\sigma} \cdot \boldsymbol{n} = \boldsymbol{0}$$ “free surface”

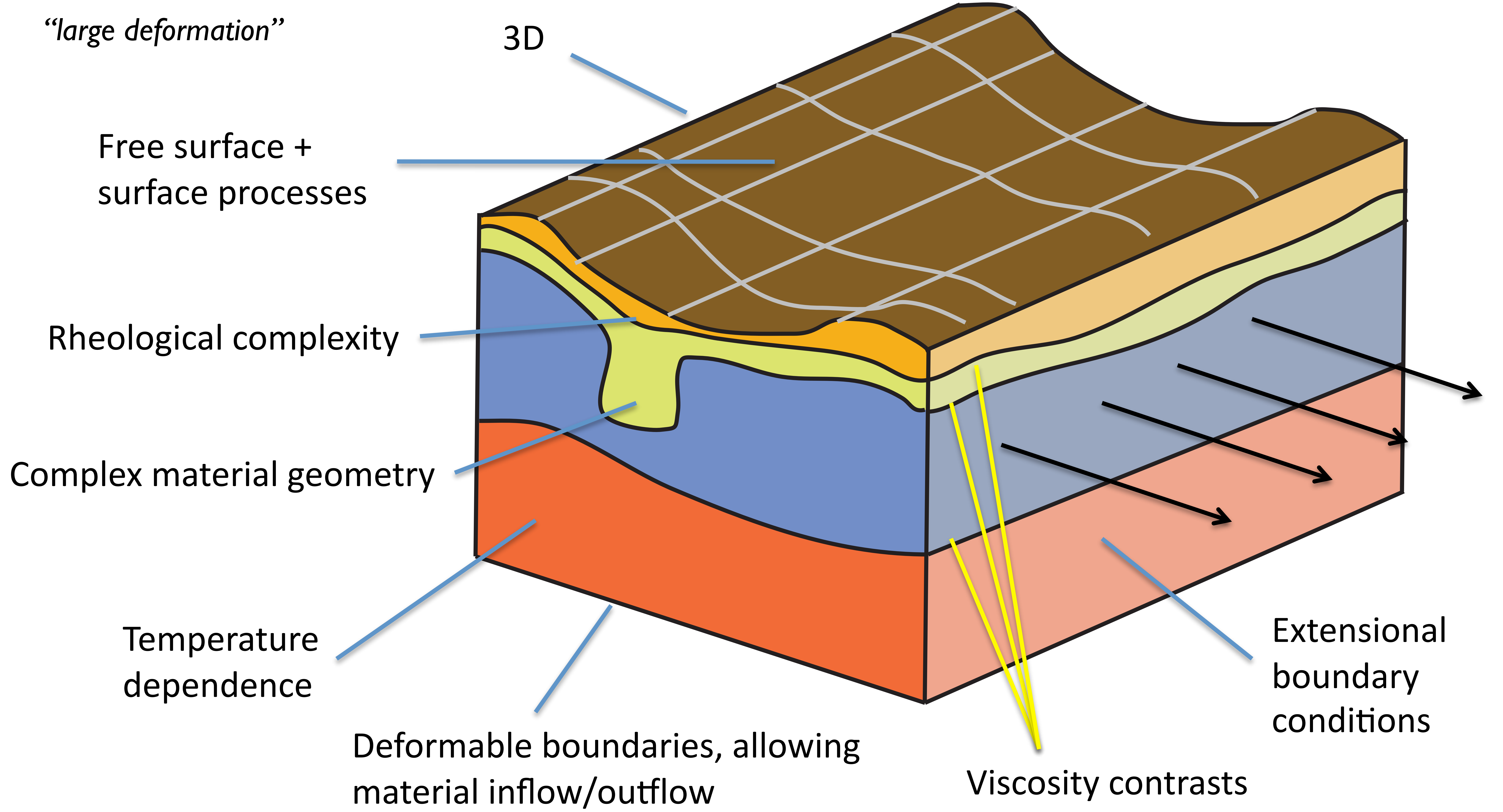


$$T = T_D$$ temperature Dirichlet

$$-k\nabla T \cdot \boldsymbol{n} = 0$$ zero heat flux

$$\psi = \psi^{\text{in}}, \text{where } \boldsymbol{u} \cdot \boldsymbol{n} < 0$$ material inflow

A “minimum” complexity model



General numerical modelling approach

- Define a geodynamic model.
- Decompose the physical domain into pieces (cells or vertices). This will define a mesh.
- Initialize the discrete model inputs.
- for each increment in time
    1. Discretize the governing equations in space (and time) over each piece in the mesh. At this point you have turned your continuous PDE into a system of discrete equations.
    2. Solve for the discrete velocity, pressure, temperature.
    3. Advect rock type / composition using the computed velocity.

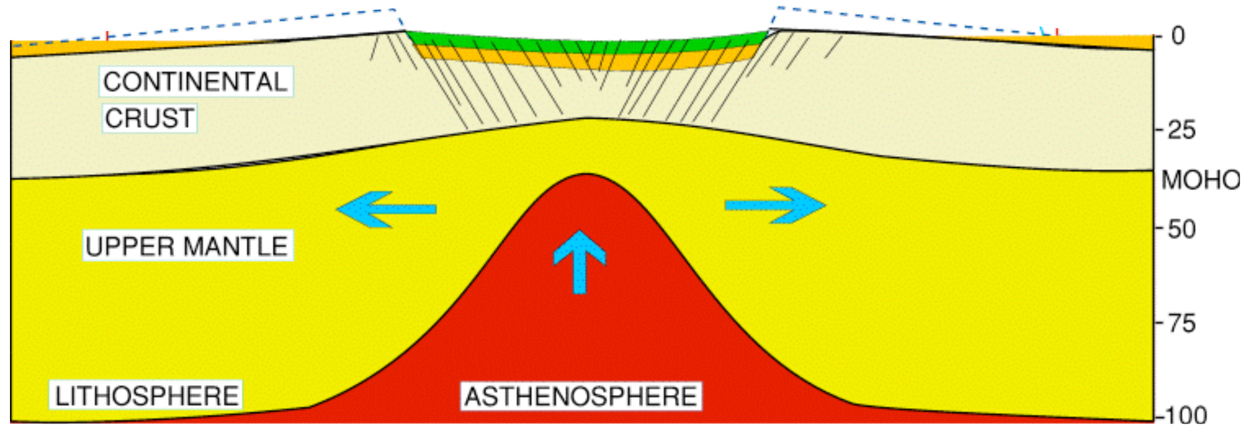
Geodynamic modelling method of choice

- Material Point Method

- Use two different spatial discretizations

  - Composition / rock type —> Lagrangian particles

  - Velocity, pressure, temperature —> grid



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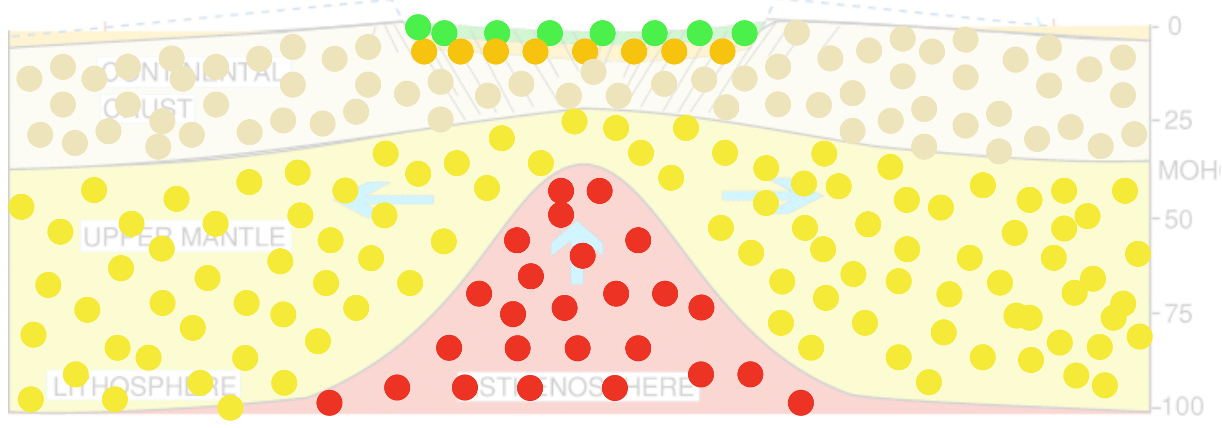
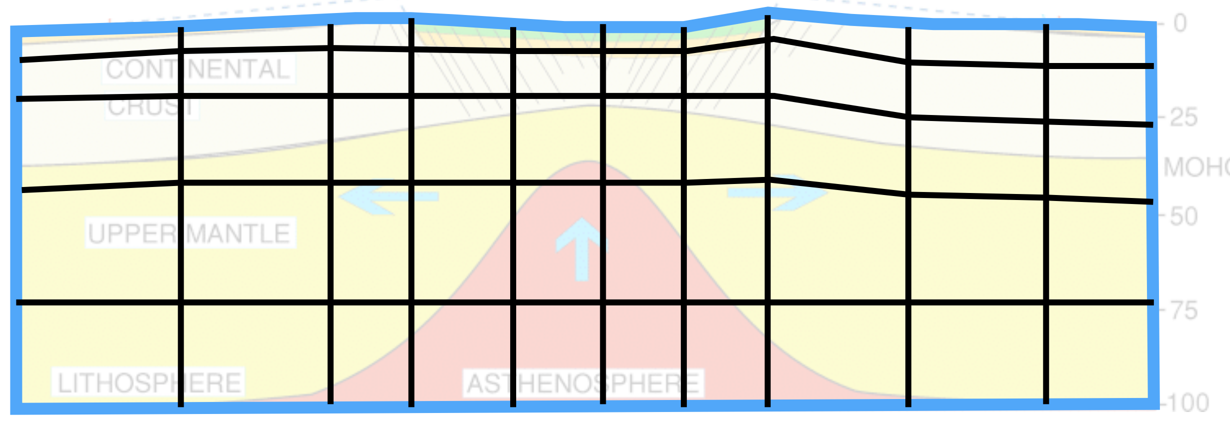
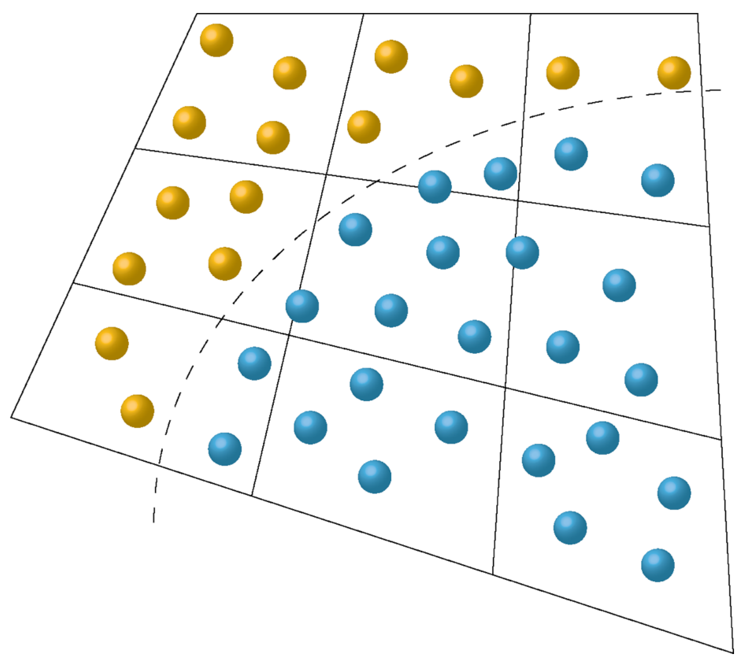
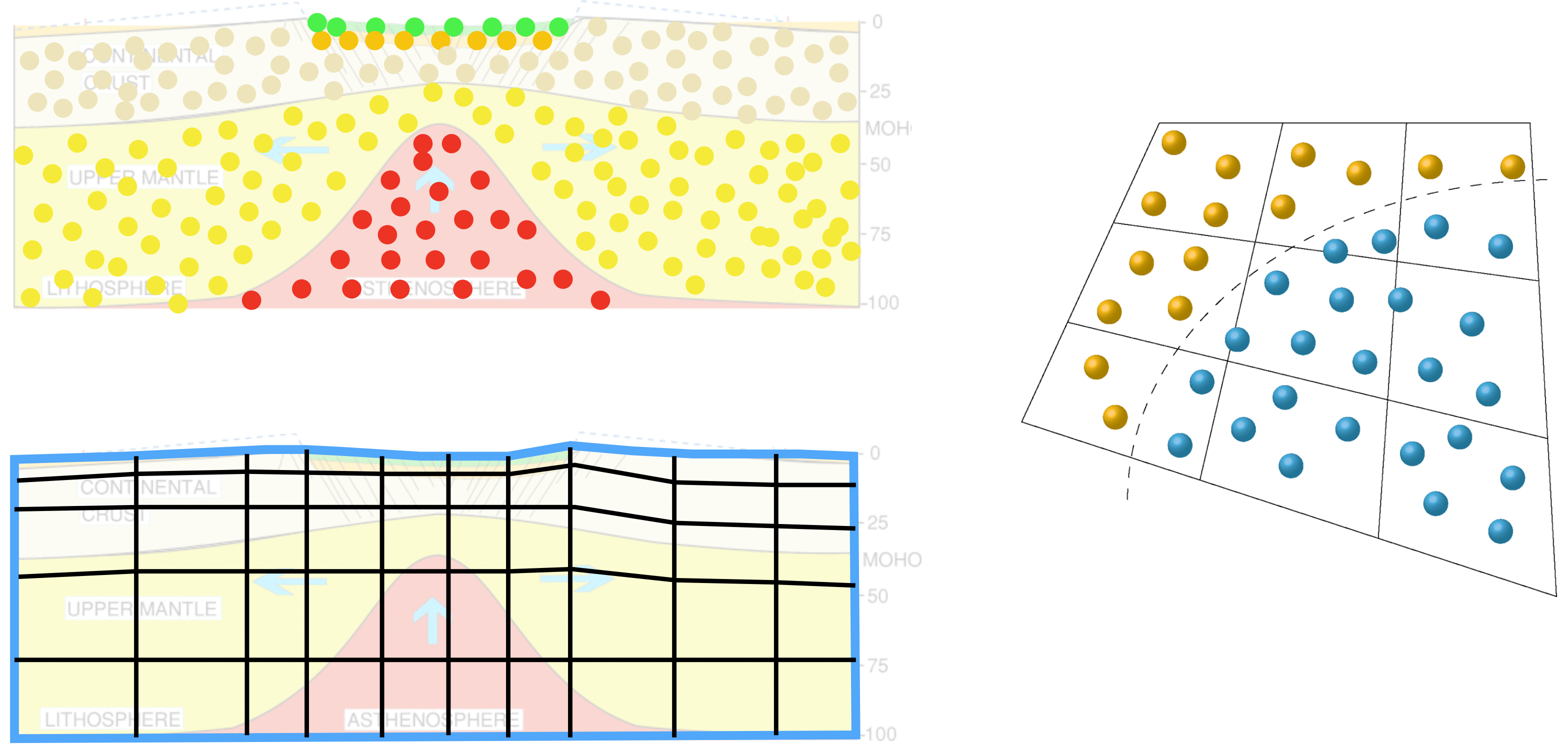




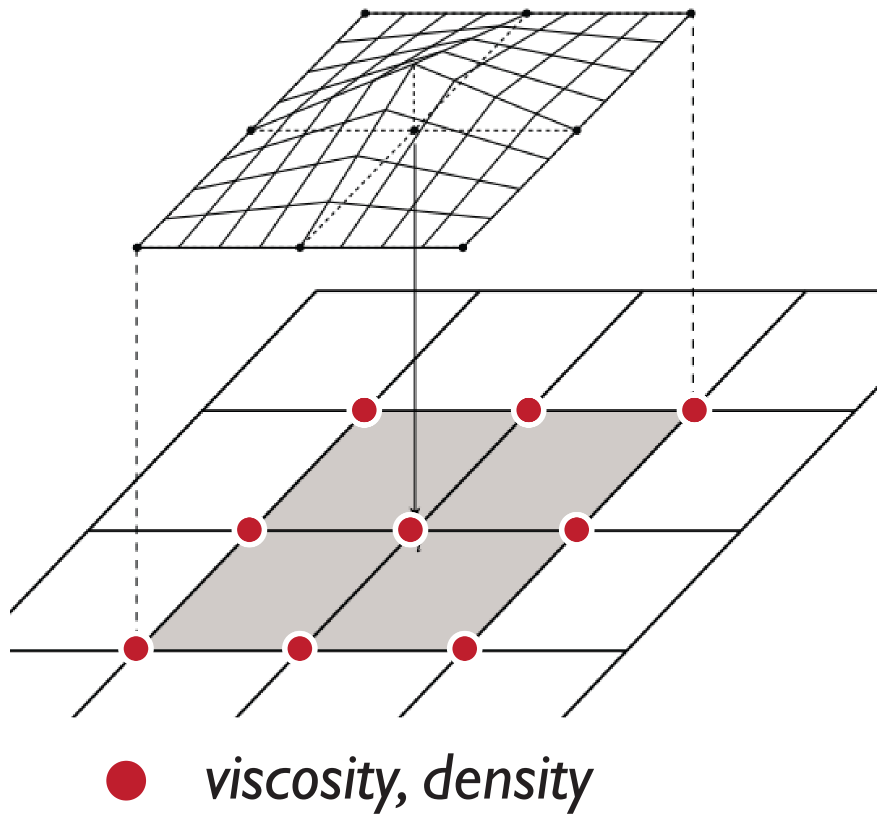


Geodynamic modelling method of choice

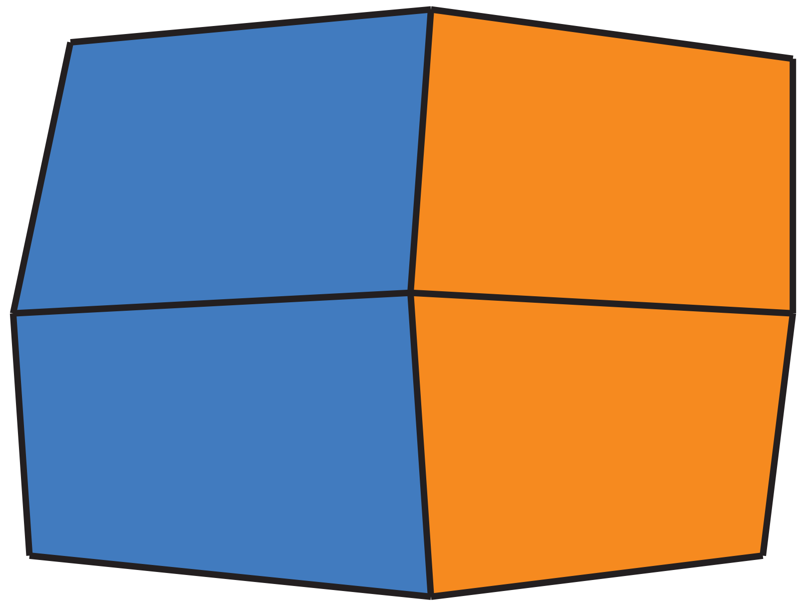
- <u>Material Point Method</u>
- **Lagrangian particles**
    - Store history variables (stress, damage) and material type
    - Advected through the mesh
- Reconstruct coefficients (e.g. viscosity)



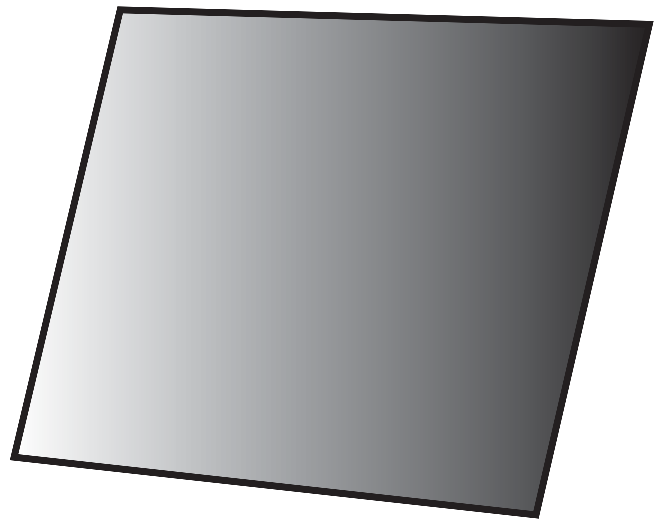
[a] Local L2 projection (Q1)



[b] Piecewise constant (P0)



[c] Piecewise linear (P1)



Material Point Method

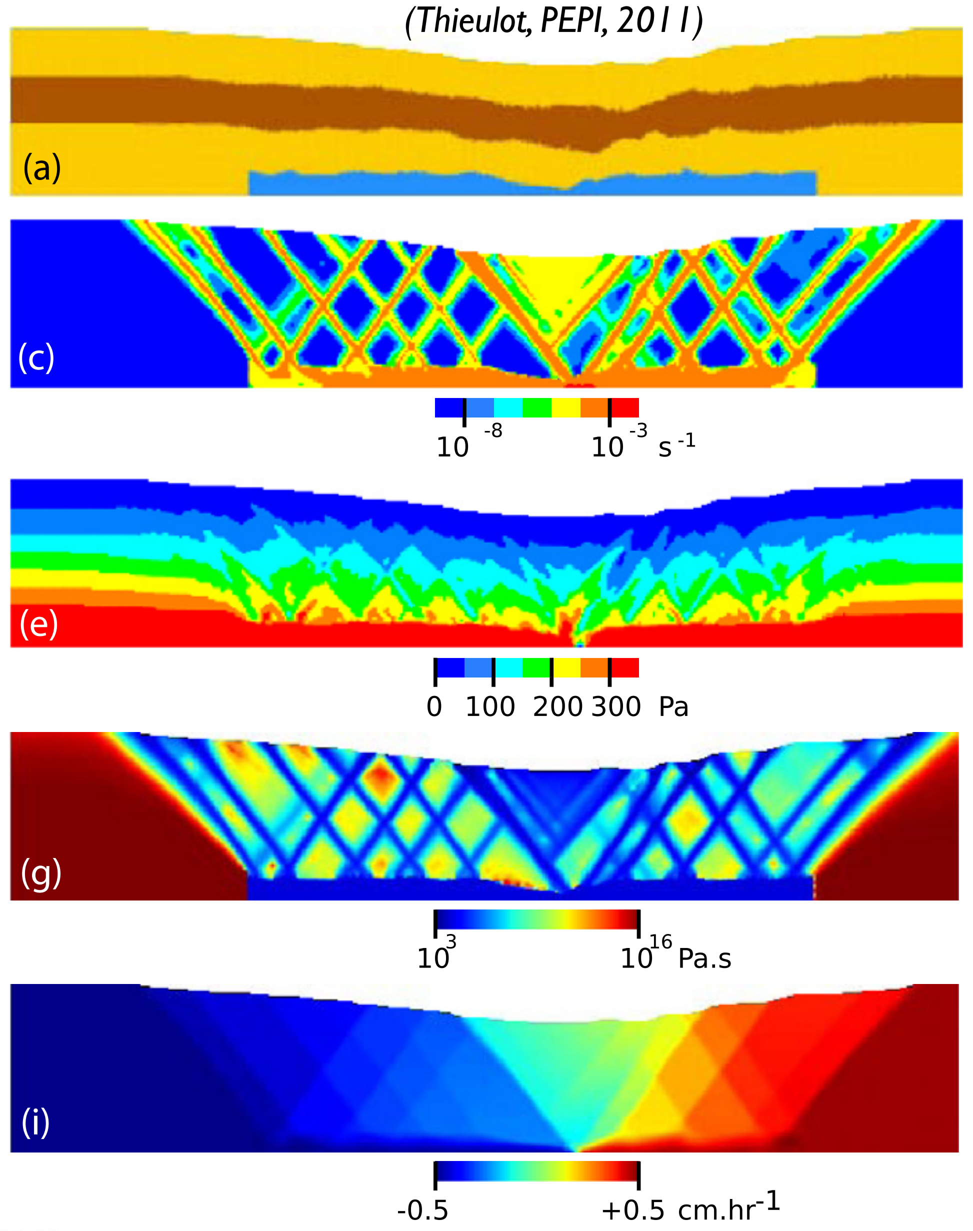
Finite element variants

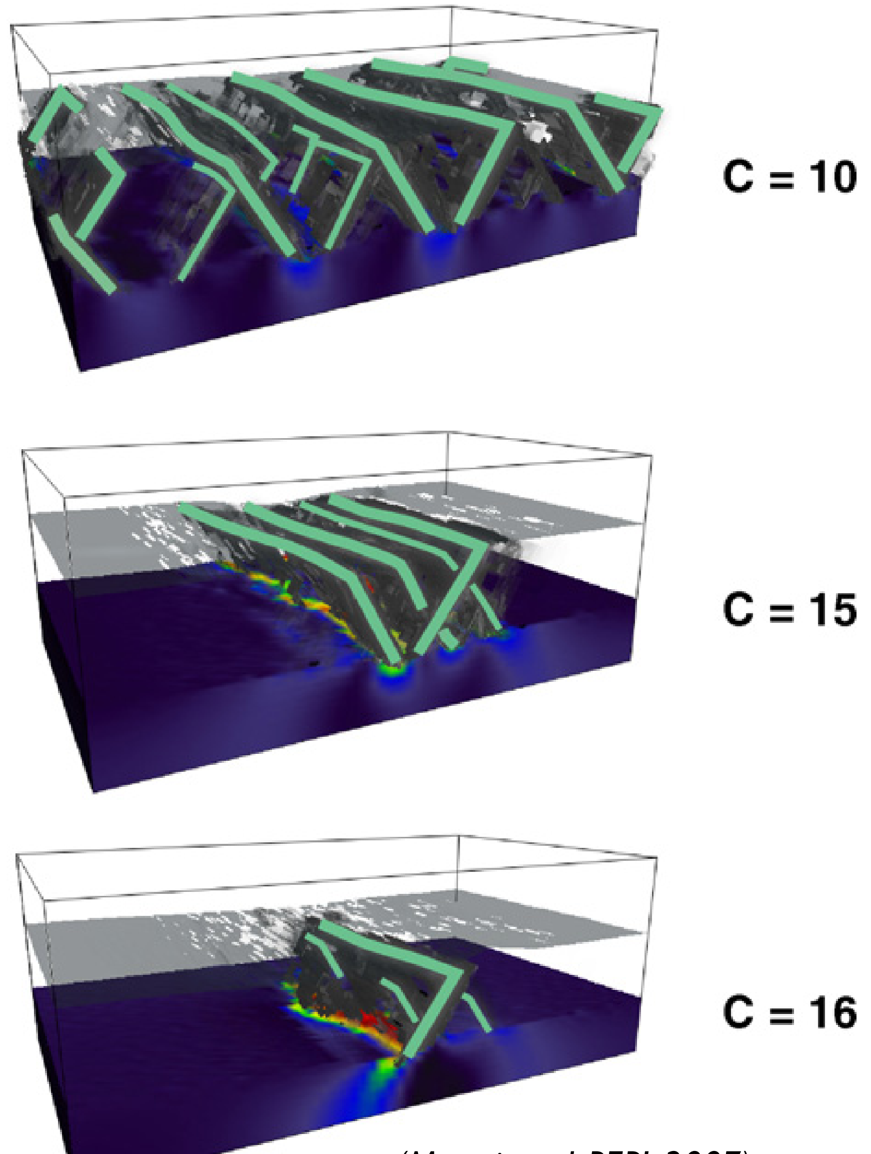
- PARAVOZ / FLAMAR [Podladchikov, Burov, 1993]
- SOPALE [Fullsack, 1995]
- Underworld / GALE [Moresi, 2003]
- DOUAR [Braun, 2008]
- SLIM3D [Popov, 2008]
- FANTOM [Thieulot, 2011]
- ELEFANT [Thieulot, 2013]
- pTatin3d [May, 2014]
- MILAMIN [Dabrowski, 2008]

Finite difference variants

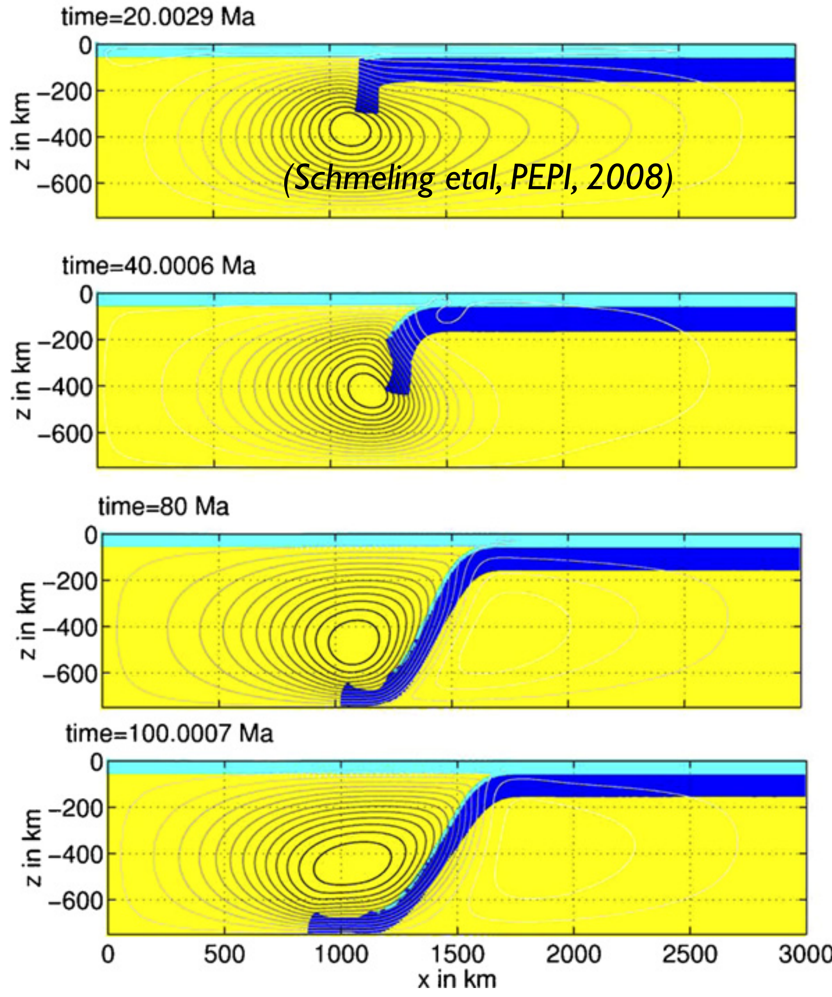
- I2VIS / I3VIS [Gerya, 2003]
- LaMEM [Kaus, 2014]

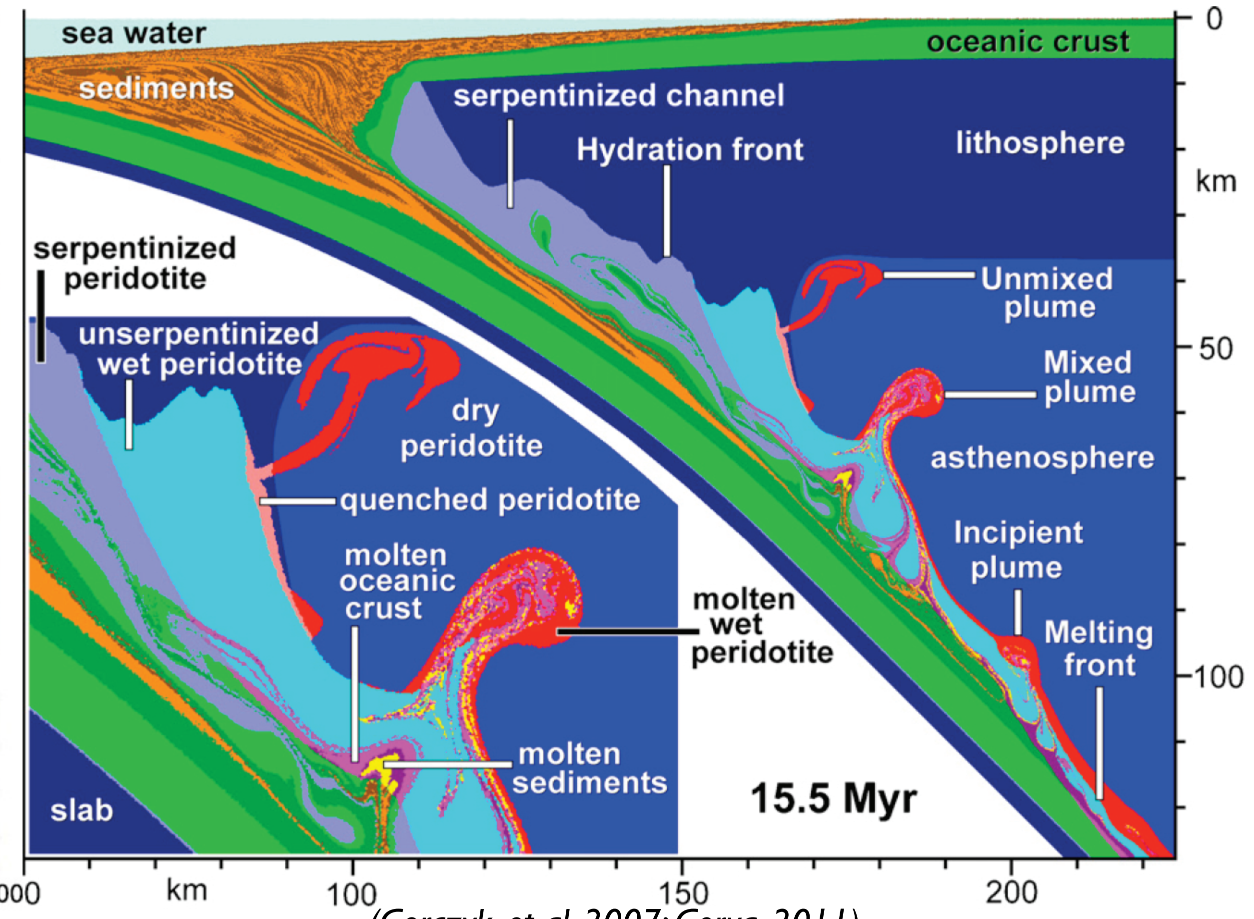
(Thieulot, PEPI, 2011)





(Moresi et al, PEPI, 2007)





(Gorczyk, et al, 2007; Gerya, 2011)

Grid based spatial discretizations

- Two most popular approaches
  - Staggered-grid Finite Difference (StagFD) method
  - Mixed Finite Element (FE) method

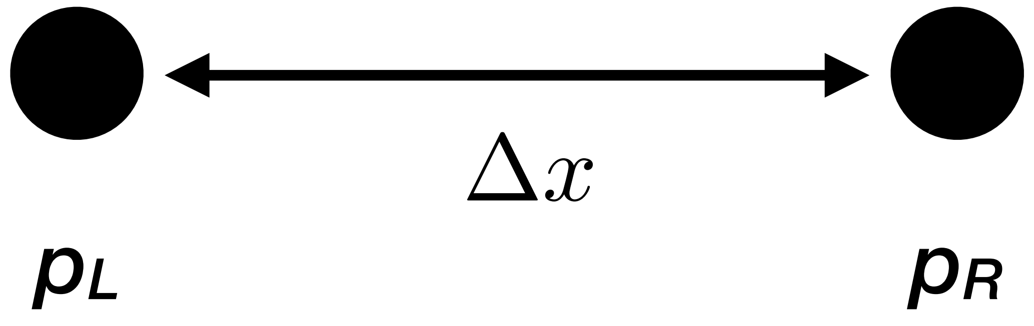
- We will overview both approaches applied to solve the viscous flow problem

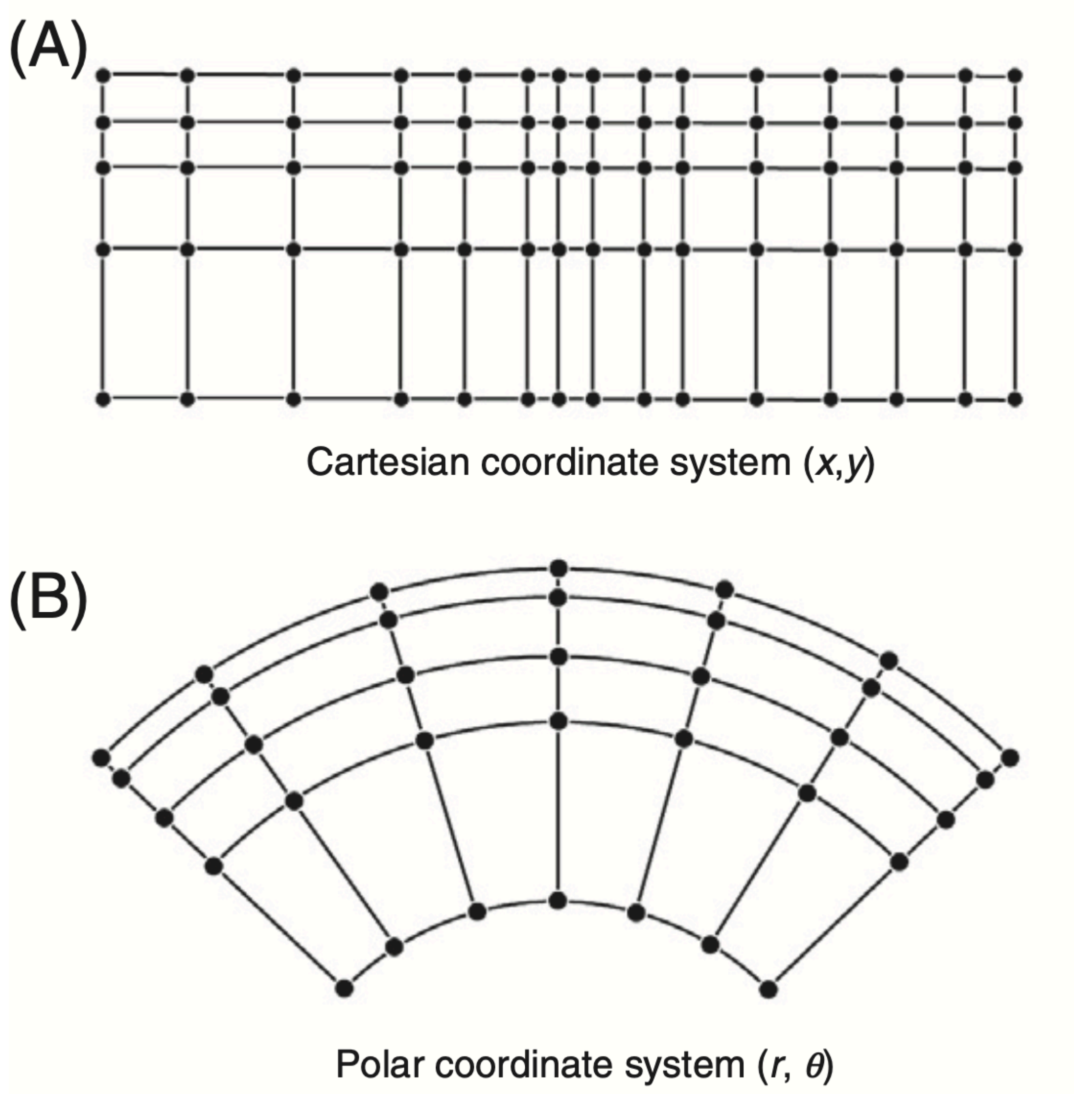
$$
\begin{aligned}
\nabla \cdot \left(\eta(\nabla u + \nabla u^T)\right) - \nabla p = f \\
\nabla \cdot u = 0
\end{aligned}
$$

Finite Differences

- Fundamental building blocks
  - All partial derivatives can be approximated via differencing between neighbouring points.
  - Simple difference approximation leads to the requirement of a structured grid, moreover a grid defined by an orthogonal coordinate system.
  - Apply the finite difference approximation to all terms in the governing equation, and apply to all grid points in the mesh.

$$\frac{\partial p}{\partial x}(x^*) \approx \frac{p_R - p_L}{\Delta x}$$





Staggered-grid Finite Differences

- Special layout of variables for the x, y components of velocity and pressure (and more)

$$\nabla \cdot (\eta(\nabla u + \nabla u^T)) - \nabla p = f$$
$$\nabla \cdot u = 0$$

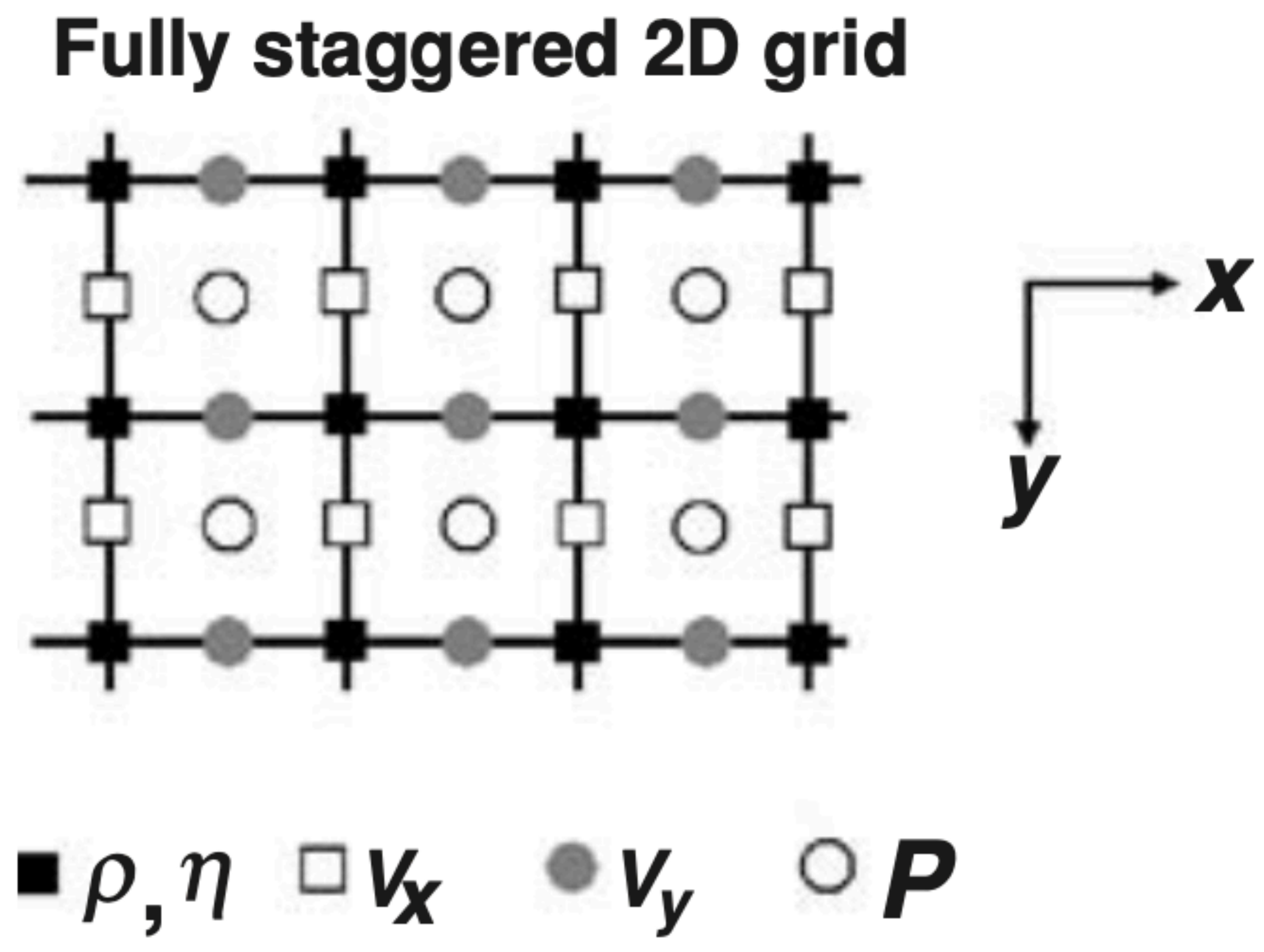
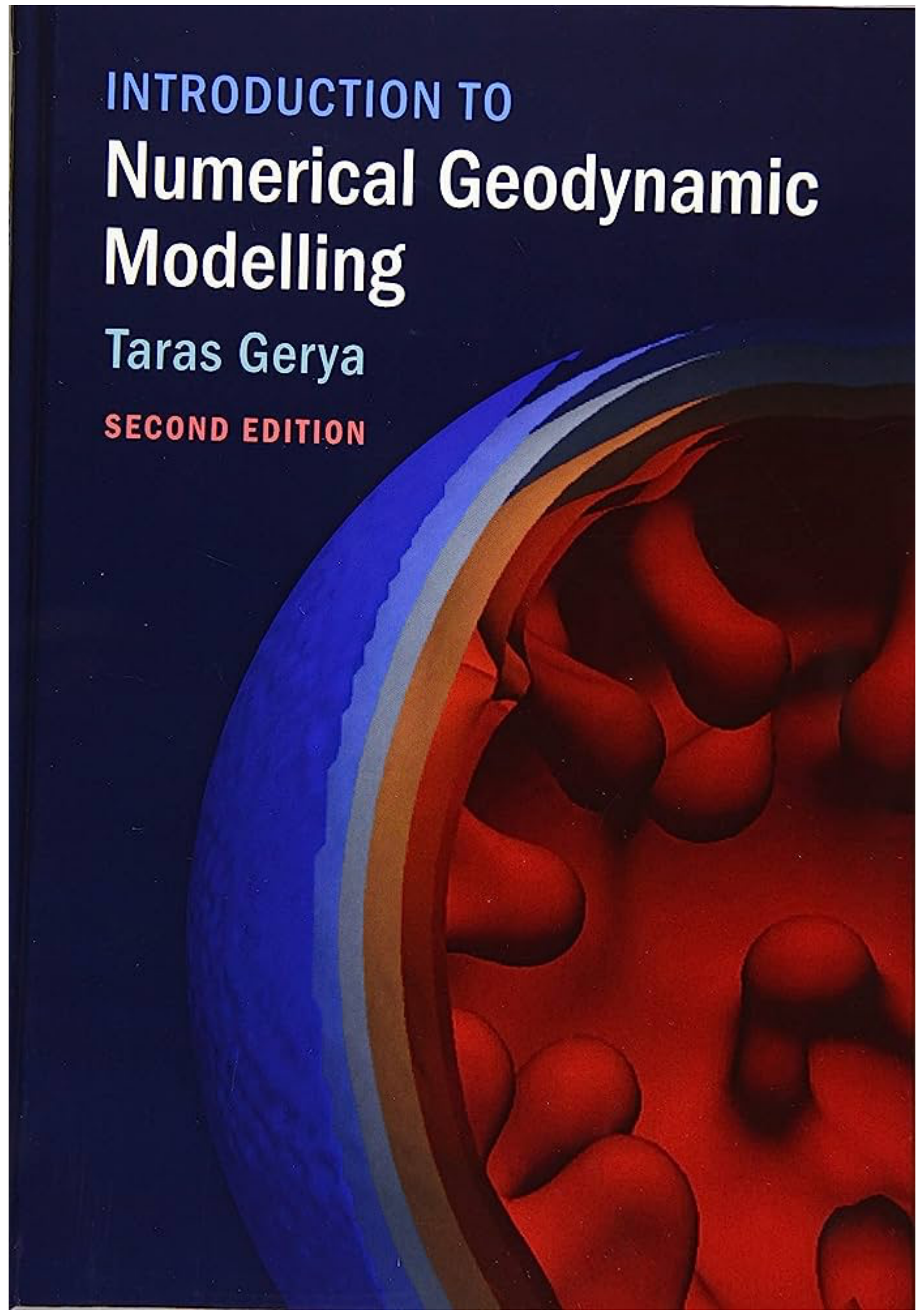


Fig. 7.7 Example of a fully staggered 2D numerical grid.



Staggered-grid Finite Differences

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$$\nabla \cdot (\eta(\nabla u + \nabla u^T)) - \nabla p = f$$
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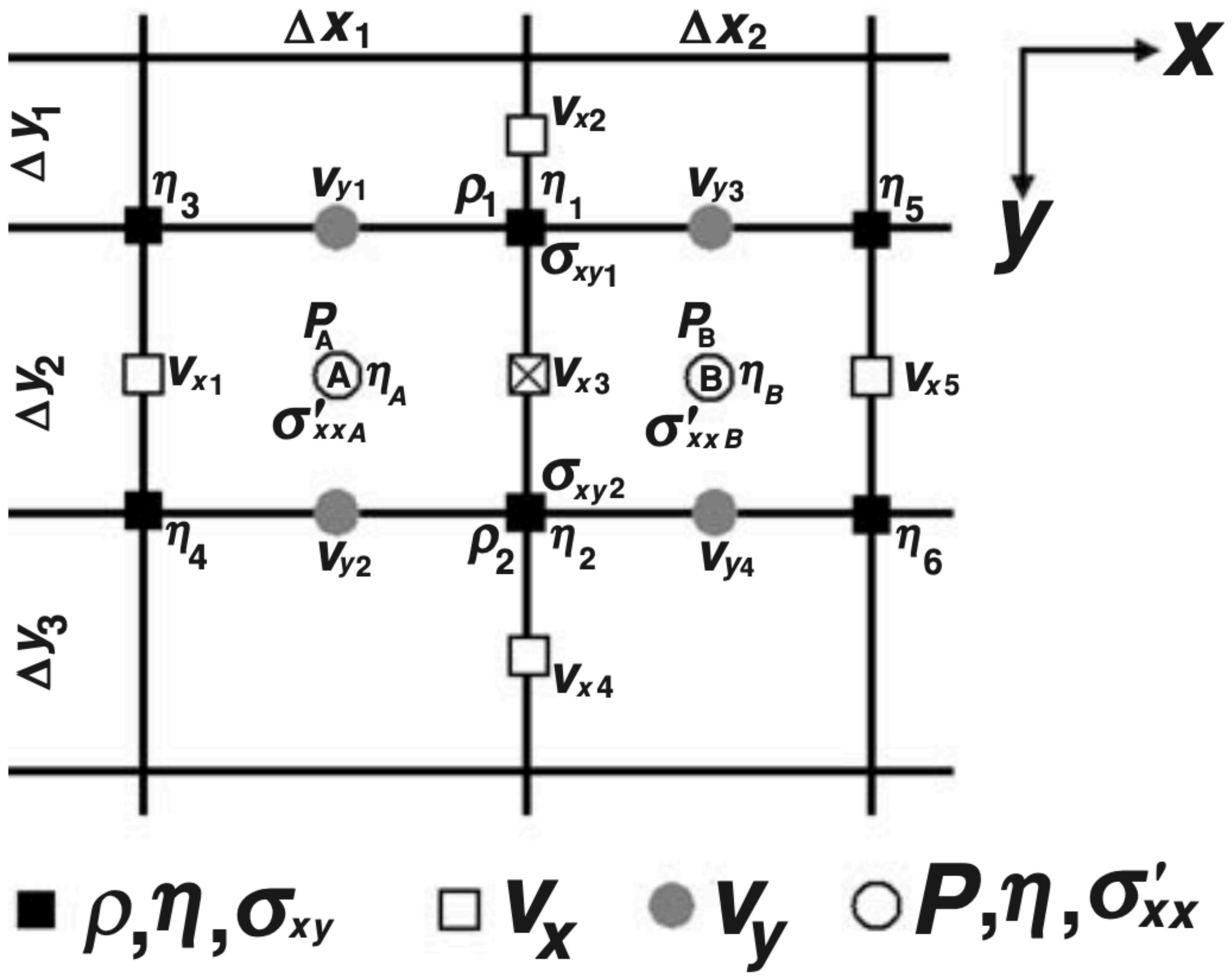
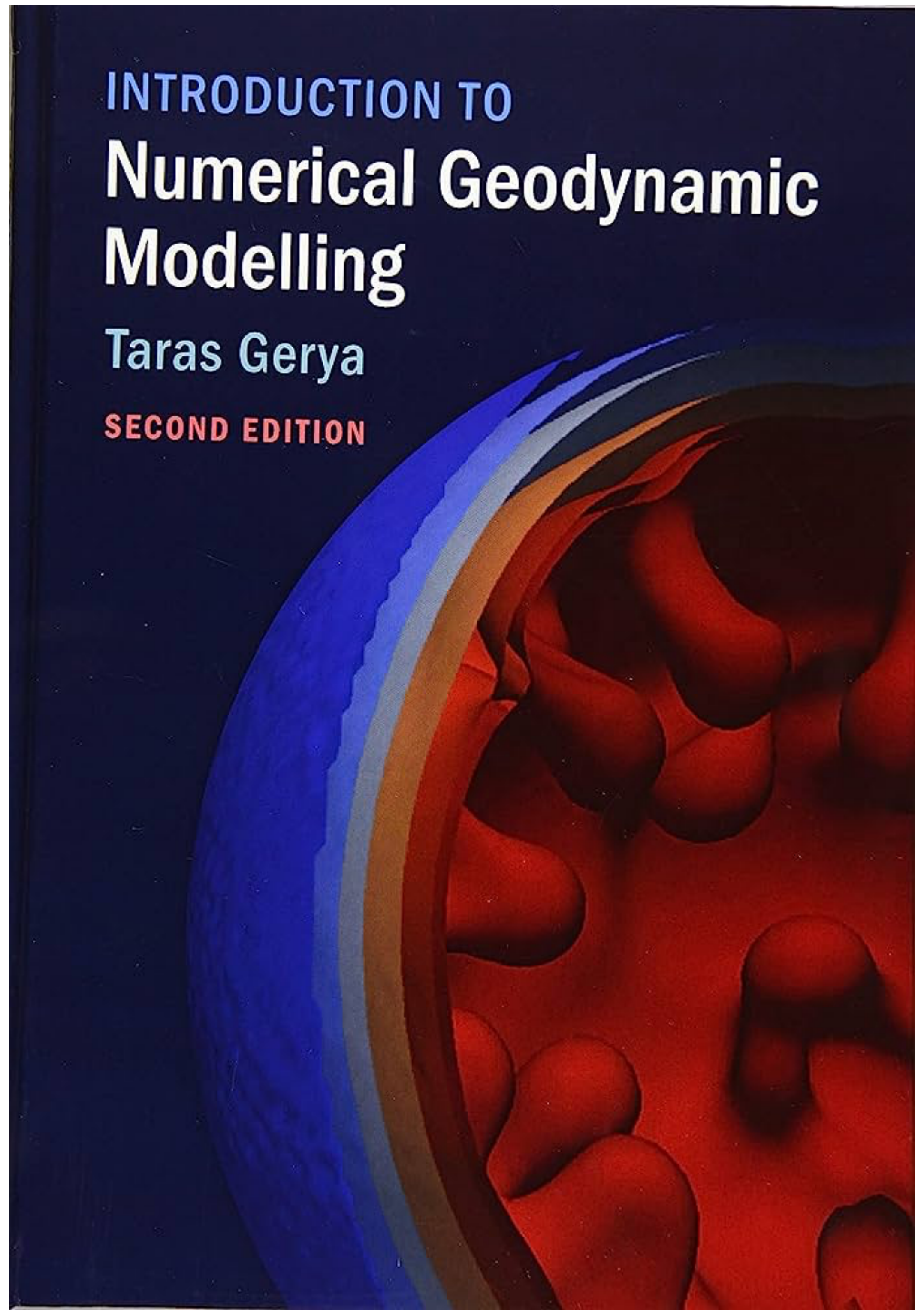


Fig. 7.11 Stencil of a 2D staggered grid used for discretisation of x-Stokes equation with a variable viscosity. The crossed square corresponds to the node at which the x-Stokes equation is formulated.



Advantages

- Conservative.
- Suitable for 2D and 3D.
- Very few degrees of freedom (unknowns).
- Few unknowns —>
  - low memory required .
  - fast to compute solutions.
- Robust with respect to the model configuration.

Disadvantages

- Evaluating the discrete solution (or its gradient) at arbitrary locations in the mesh is not natural.
- Imposing Dirichlet and Neumann (natural) boundary conditions is not completely natural.
- Geometrically inflexible.
  - Free surface evolution is not natural.
- Extensions to other governing equations, and or coupling with other governing equations is not always straight forward.
- Generic software implementations are challenging.
- Non-linear problems result in stencil growth.

Finite Element Method

- Fundamental building blocks
  - Seeks solutions to the weak form.
  - Spatial domain decomposed into cells (finite elements).
  - Approximate unknown field (e.g. T) by a cell-wise defined polynomial.

Find u such that

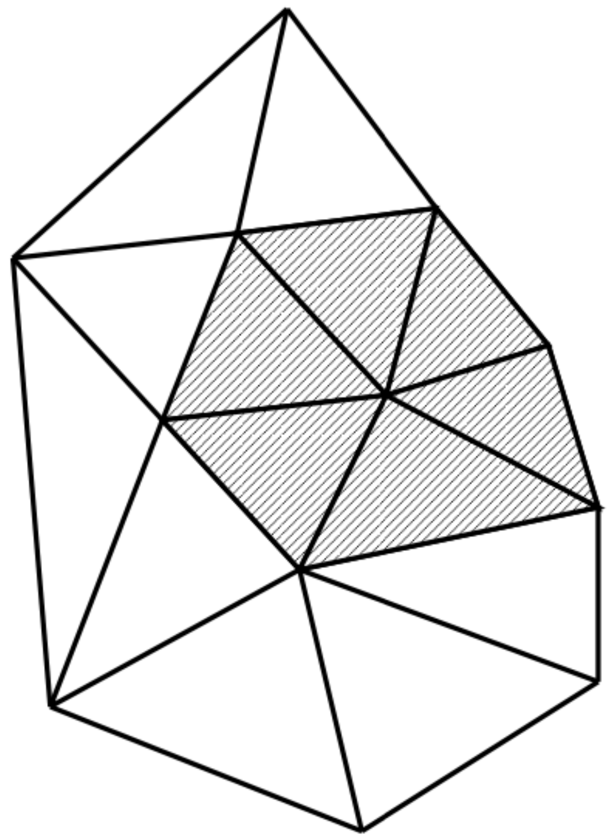
$$-\nabla^2 u = f \quad \text{in } \Omega \tag{1.13}$$

$$u = g_D \text{ on } \partial\Omega_D \quad \text{and} \quad \frac{\partial u}{\partial n} = g_N \text{ on } \partial\Omega_N, \tag{1.14}$$

where $\partial\Omega_D \cup \partial\Omega_N = \partial\Omega$ and $\partial\Omega_D$ and $\partial\Omega_N$ are distinct.

Find $u \in \mathcal{H}^1_E$ such that

$$\int_\Omega \nabla u \cdot \nabla v = \int_\Omega v f + \int_{\partial\Omega_N} v g_N \quad \text{for all } v \in \mathcal{H}^1_{E_0}. \tag{1.17}$$



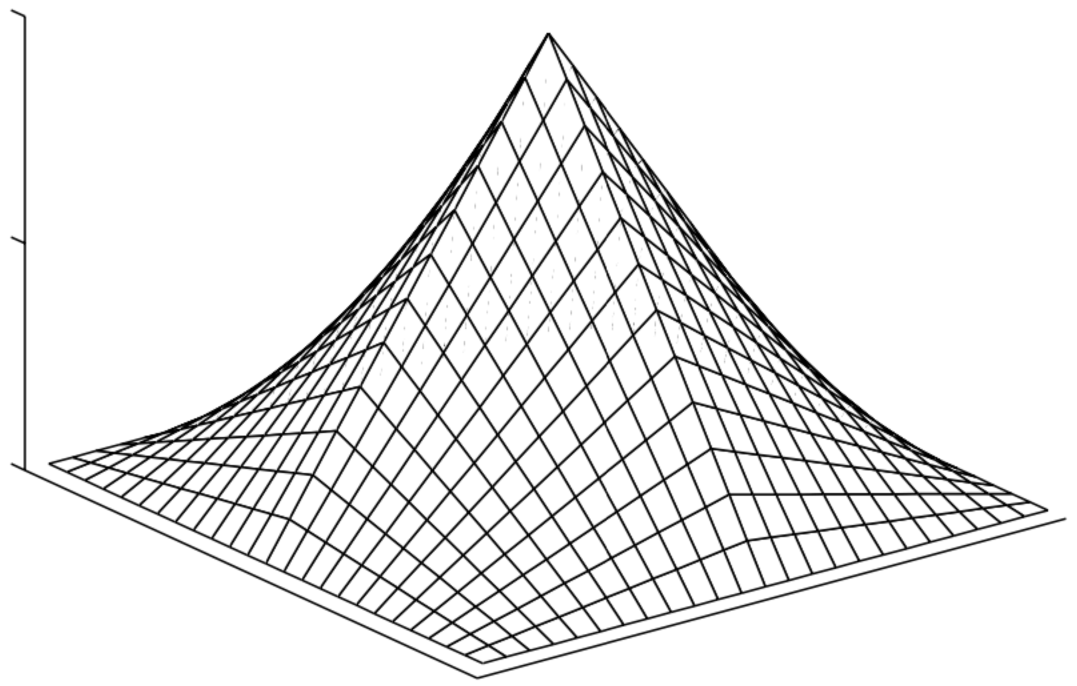
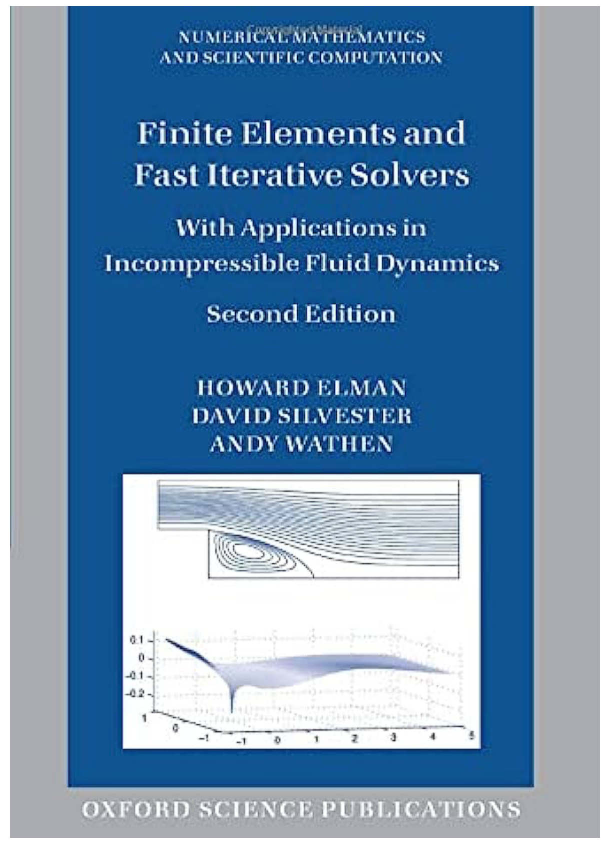
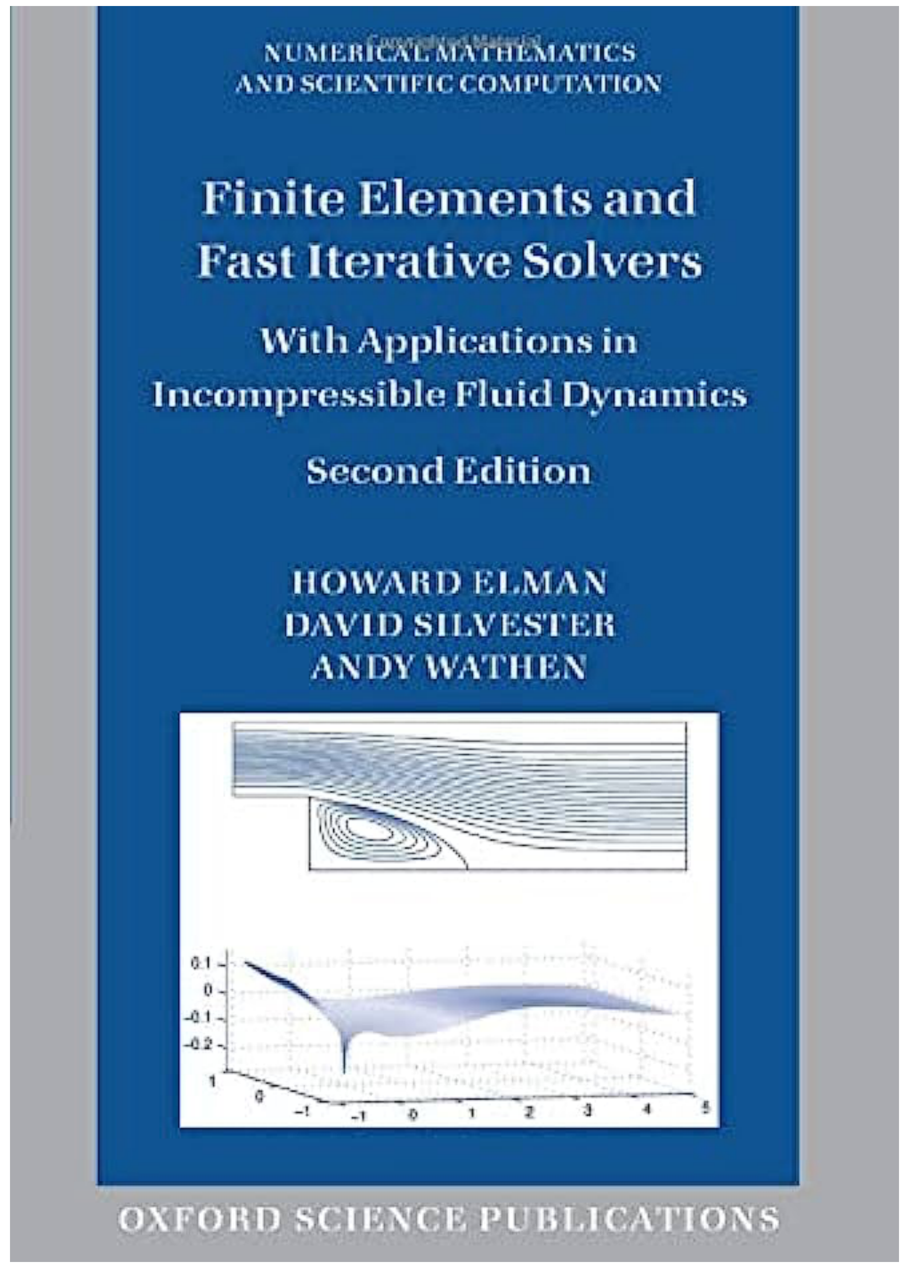


FIG. 1.9. A typical $\boldsymbol{Q}_1$ basis function.



Mixed Finite Elements

- Discretize velocity and pressure using different polynomials. Pressure may use a discontinuous function across elements.
- Low order elements, e.g. velocity (linear) and pressure (constant) are unstable and result in poor pressure solutions.
- Stabilization techniques often not suitable for geodynamics applications.
- Arguably the best “all round” choice is to use a quadratic polynomial for velocity and linear discontinuous polynomial for pressure



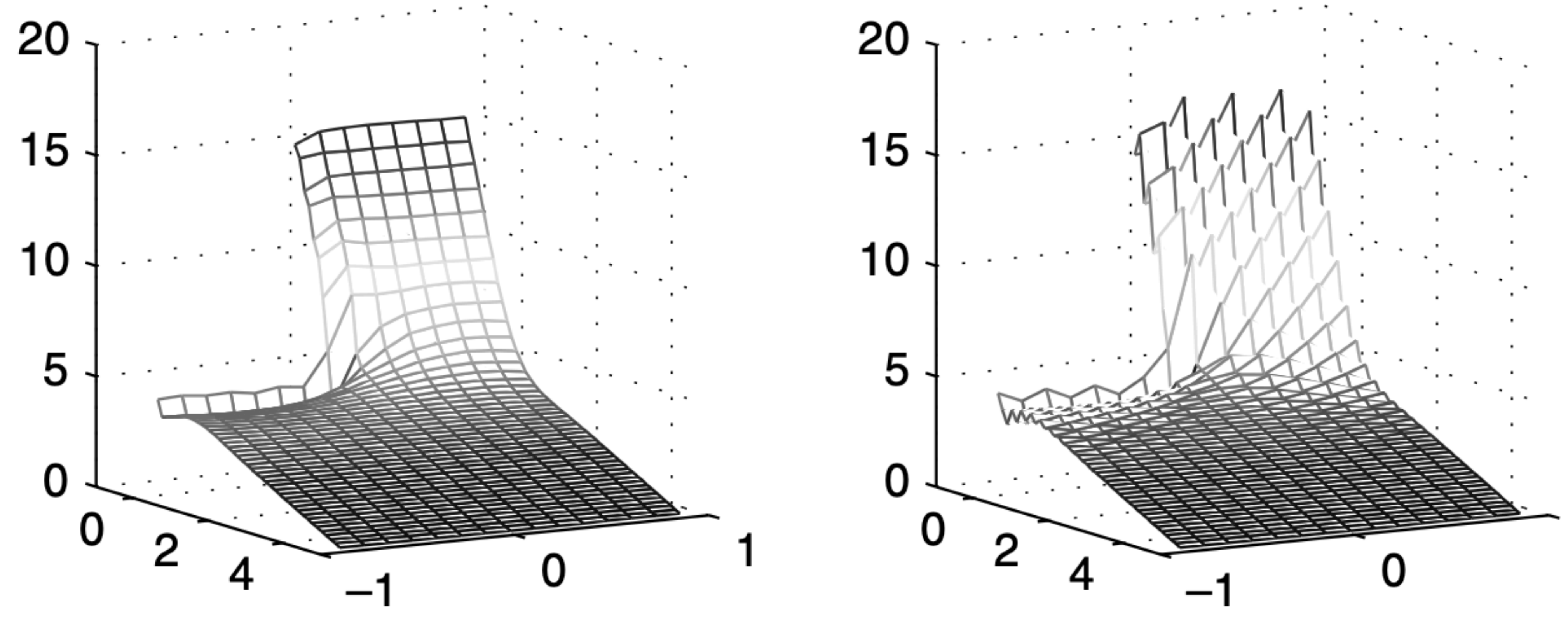
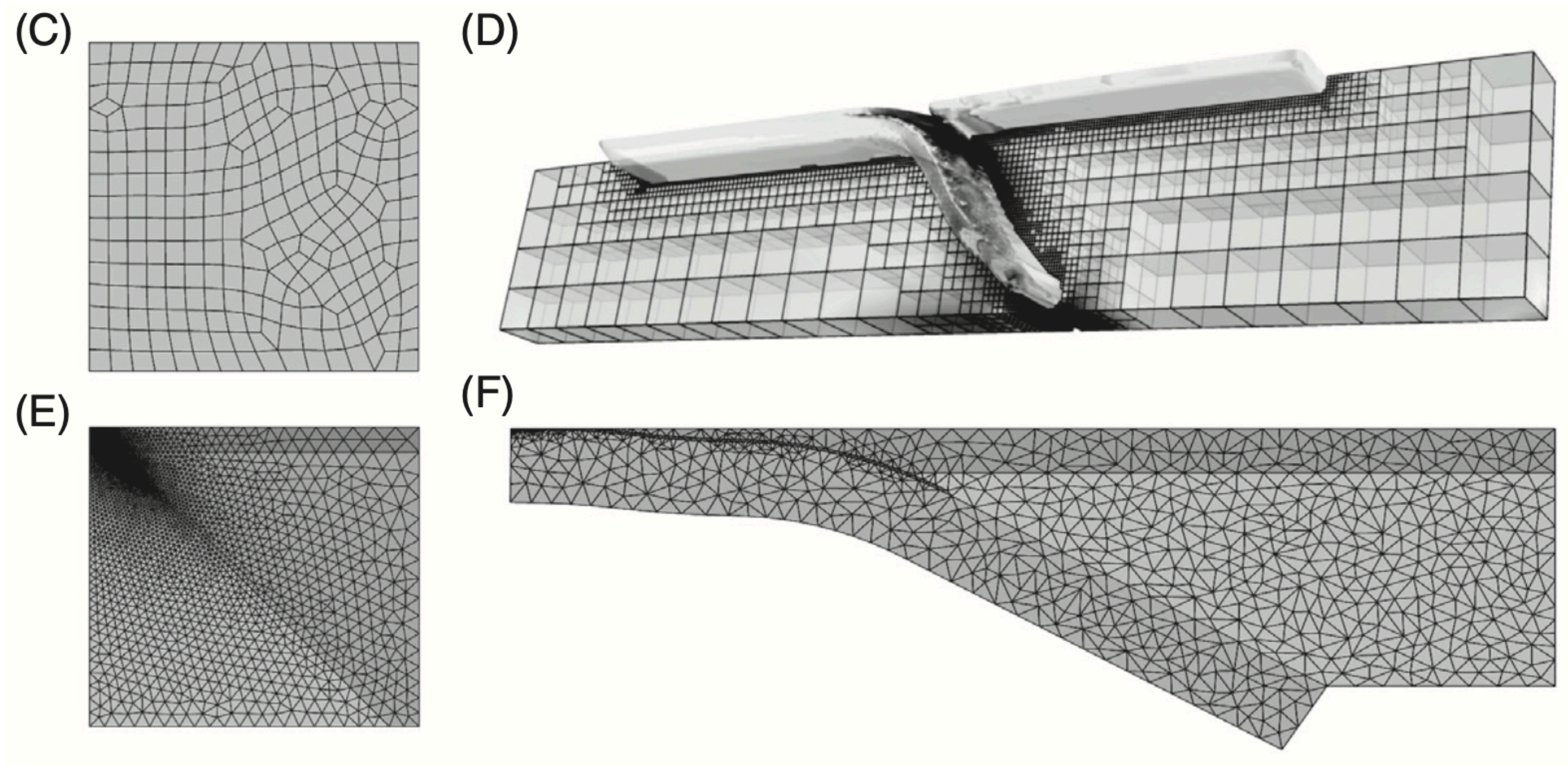


FIG. 5.13. Pressure solutions corresponding to a stabilized (left, $\beta = \beta^*$) a unstabilized (right, $\beta = 0$) $\boldsymbol{Q}_1$–$\boldsymbol{P}_0$ mixed approximation of Example 5.1.2.

Advantages

- Geometrically flexible.
  - Wide range of cell geometries and domain geometries can be used.
- Suitable for 2D and 3D.
- Imposing Dirichlet and Neumann (natural) boundary conditions is trivial.
- Suitable for problems with discontinuous coefficients
- Simple to write modular code that is extensible to new physics.
- Evaluating the discrete solution (or its gradient) at arbitrary locations in the mesh is trivial.
- Rich mathematical analysis exists.



Disadvantages

- Not naturally conservative.
- Many more degrees of freedom (unknowns) —> expensive in terms of memory and time.
- Too many element choices to think about.
- Solution stability mandates the usage of high-order (expensive) elements, however solution characteristics do not benefit from high-order accuracy.

Material Point Method

Finite element variants

- PARAVOZ / FLAMAR [Podladchikov, Burov, 1993]
- SOPALE [Fullsack, 1995]
- Underworld / GALE [Moresi, 2003]
- DOUAR [Braun, 2008]
- SLIM3D [Popov, 2008]
- FANTOM [Thieulot, 2011]
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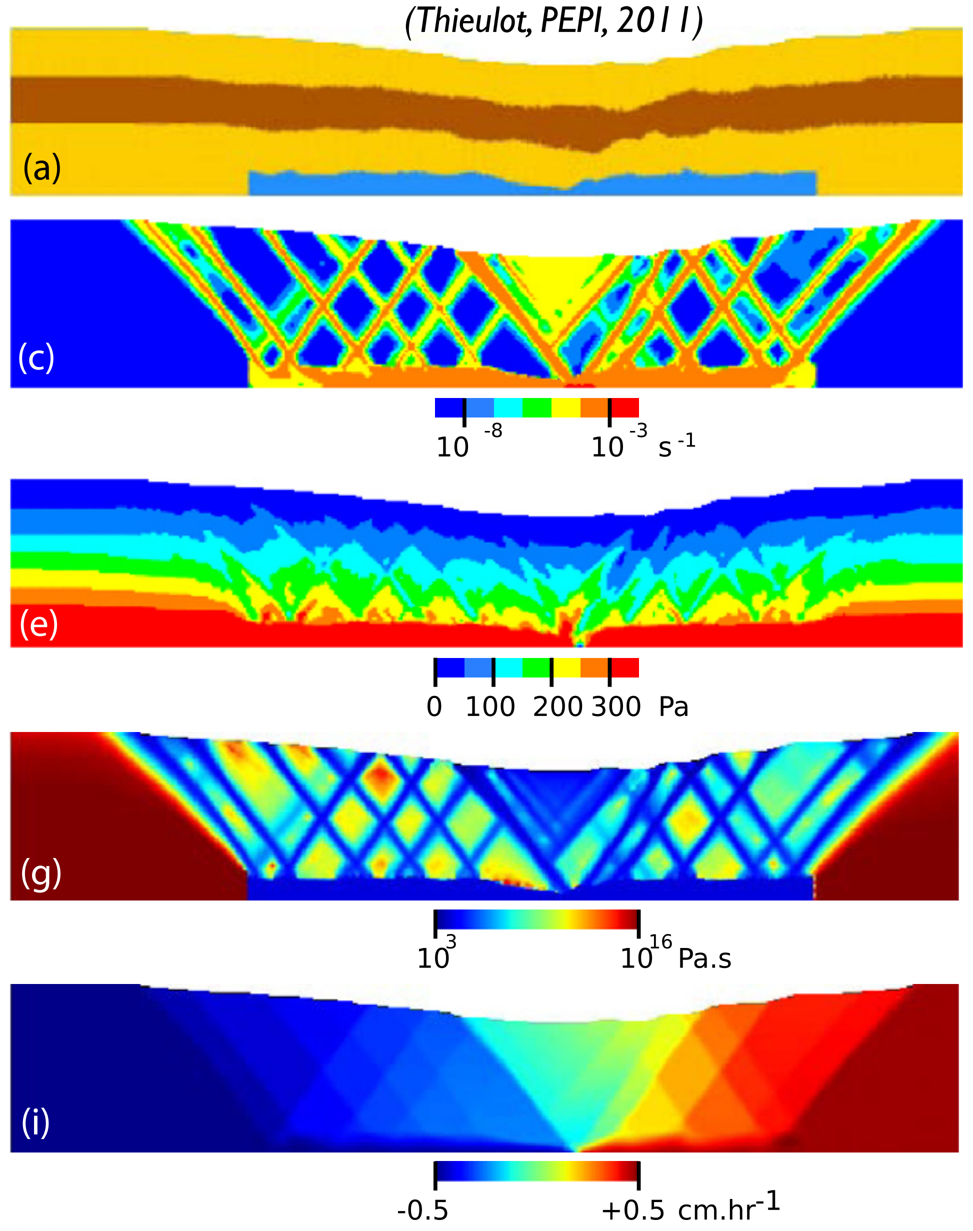
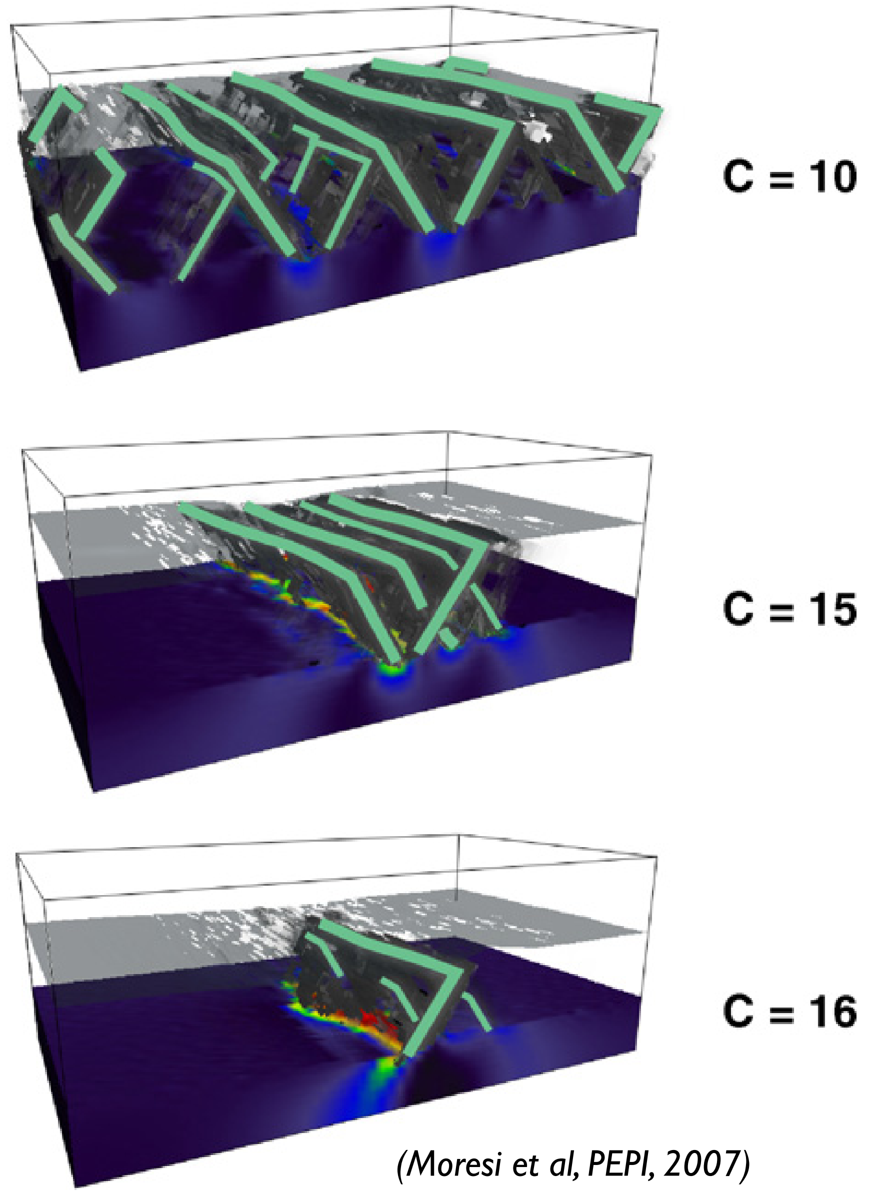
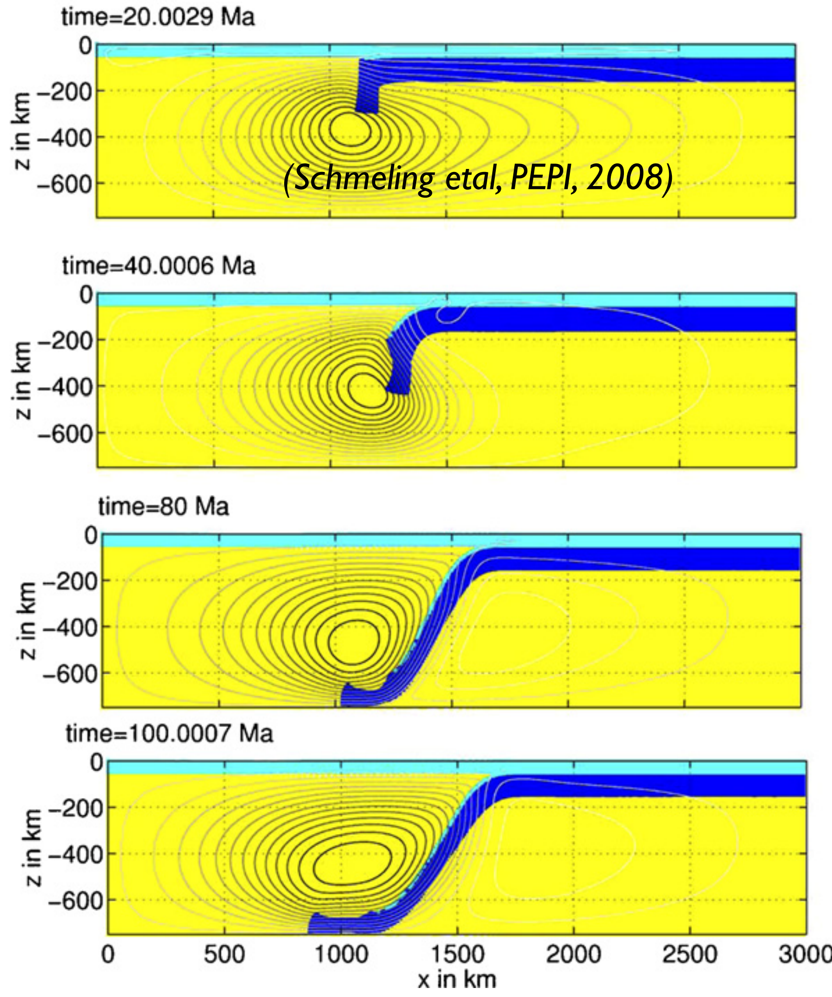
(Thieulot, PEPI, 2011)

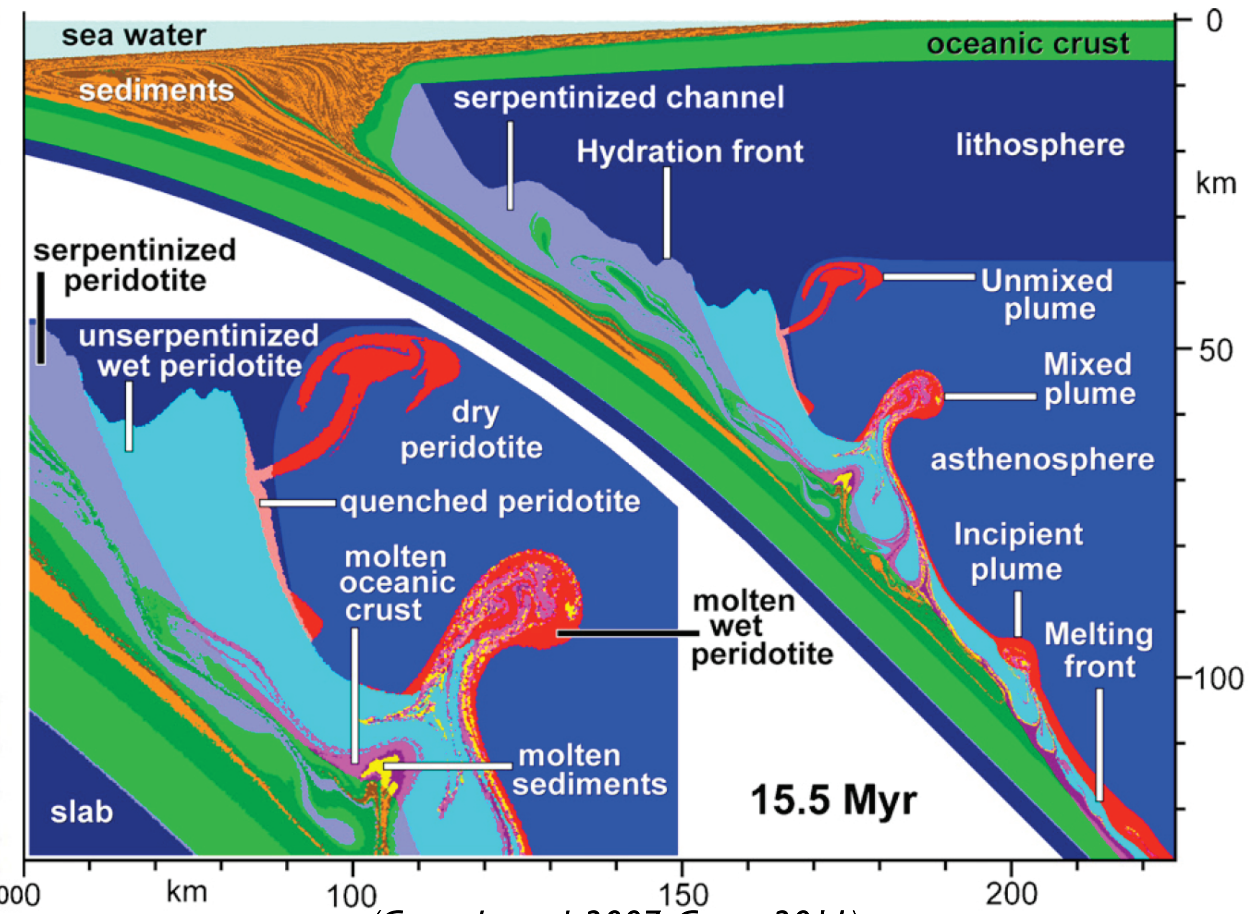




(Moresi et al, PEPI, 2007)



(Schmeling etal, PEPI, 2008)



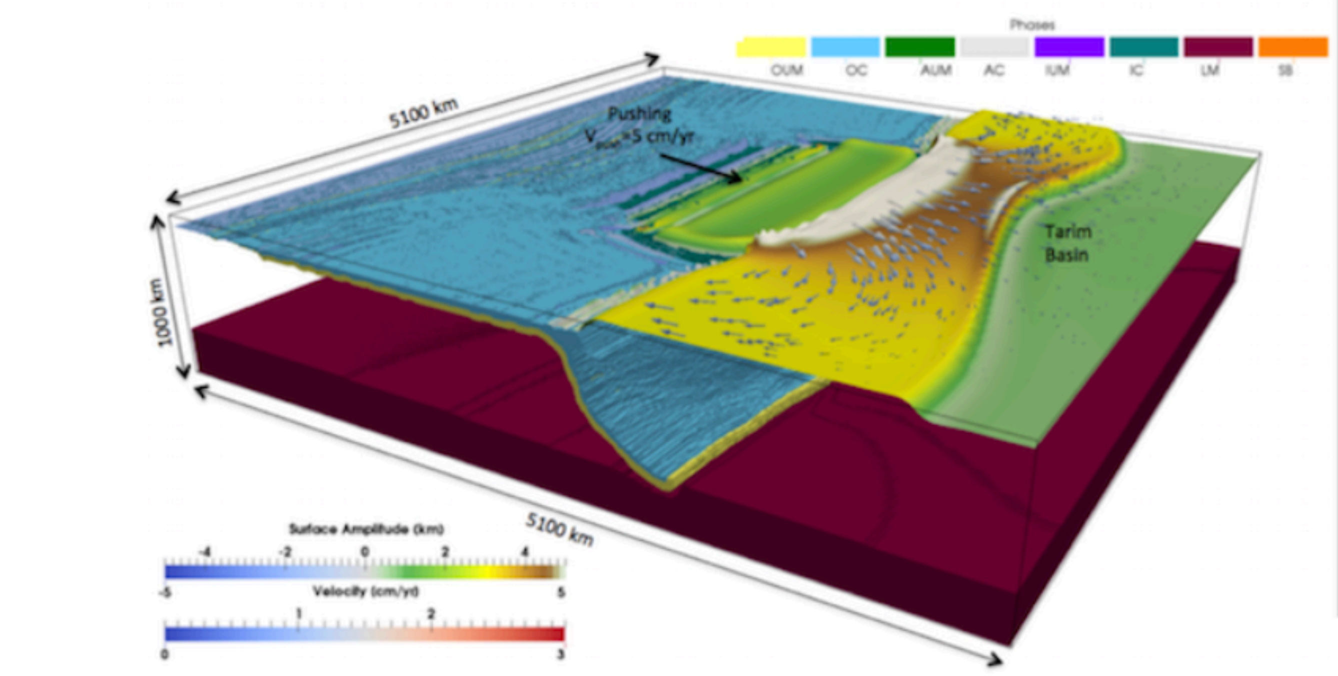
(Gorczyk, et al, 2007; Gerya, 2011)

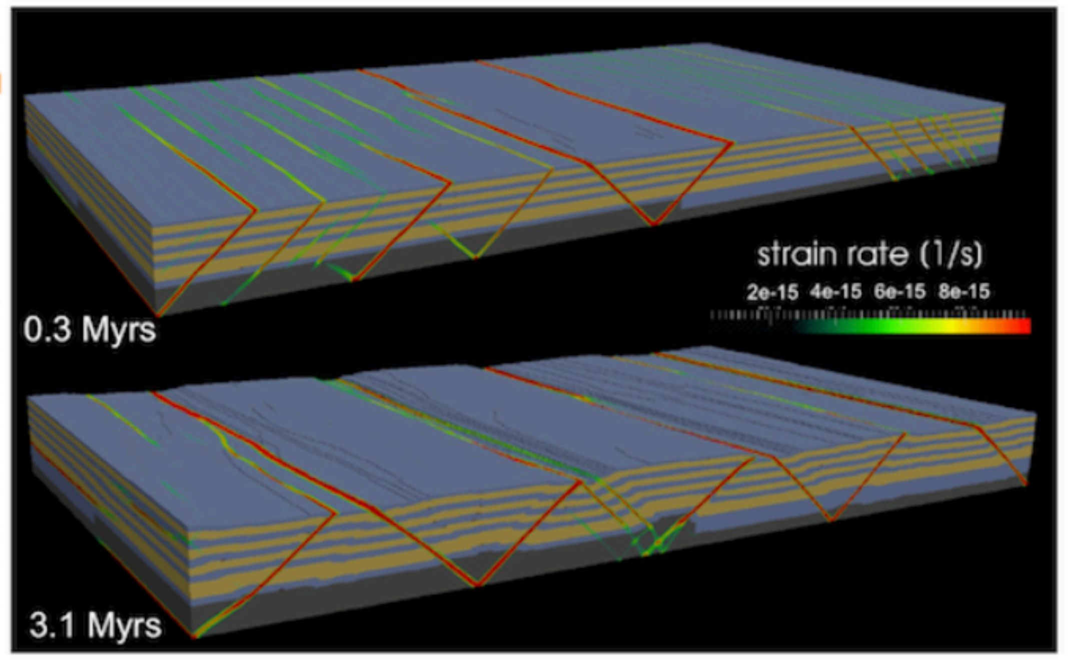
Open source geodynamic software

- LaMEM - Lithosphere and Mantle Evolution Model

- A parallel 3D numerical code that can be used to model various thermomechanical geodynamical processes such as mantle-lithosphere interaction for rocks that have visco-elasto-plastic rheologies. The code is build on top of PETSc package and the current version of the code uses a marker-in-cell approach with a staggered finite difference discretization.

LaMEM





https://github.com/UniMainzGeo/LaMEM

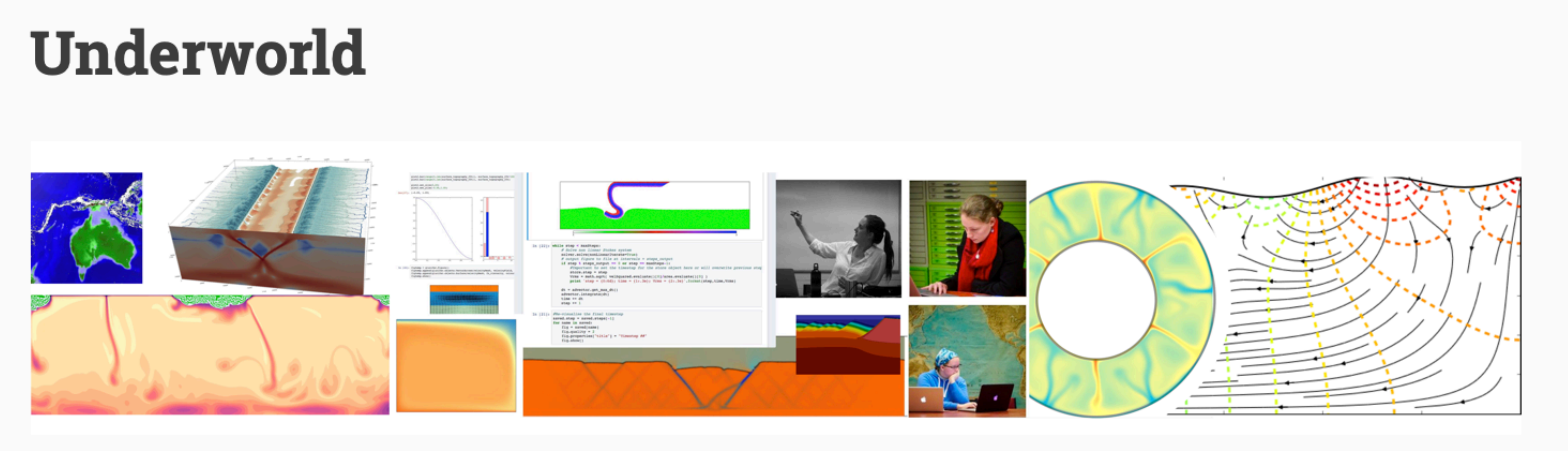
- 3D only, staggered finite difference, large scale HPC support, particles, Julia interfaces, flexible solver configuration

Open source geodynamic software

- Underworld2 is a Python API which provides functionality for the modelling of geodynamics processes. The API also provides the tools required for inline analysis and data management.

- Designed to work seamlessly across PC, cloud and HPC infrastructure.

- A primary aim of Underworld2 is to enable rapid prototyping of models, and to this end embedded visualisation (LavaVu) and modern development environments such as Jupyter Notebooks have been



https://underworld2.readthedocs.io/en/v2.14.0b/

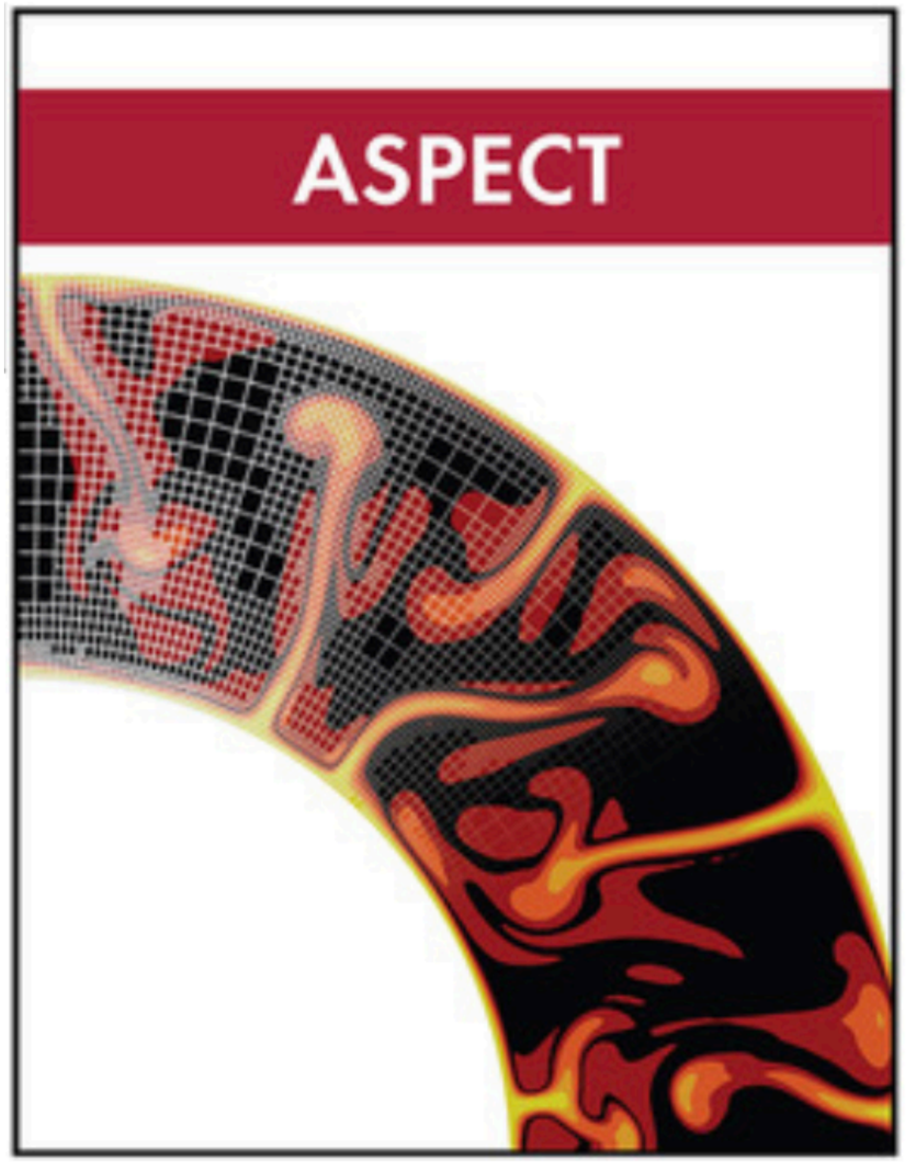
- 2D or 3D, finite elements, HPC support, particles, plug-and-play physics modules, python API to design experiments, flexible solver configuration

Open source geodynamic software

- What it is: An extensible code written in C++ to support research in simulating convection in the Earth's mantle and elsewhere.

- Mission: To provide the geosciences with a well-documented and extensible code base for their research needs.

- Vision: To create an open, inclusive, participatory community providing users and developers with a state-of-the-art, comprehensive software that performs well while being simple to extend.



https://aspect.geodynamics.org/

- 2D or 3D, finite elements, large scale HPC support, adaptive mesh refinement, particles, grid based advection, plug-and-play physics modules

Choices and tradeoffs - An example

- Is the geometry of your model domain complex?
  - Yes —> mixed FE
- Does your model require a free-surface to evolve?
  - Yes —> mixed FE
- Does you model have simple boundary conditions?
  - Yes —> StagFD
- Are your compute resources limited?
  - Yes —> StagFD

Choices and tradeoffs - An example

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- Incompatible choices may require you change your model design philosophy.
  - Think about the model problem you want to solve, then choose a method.

  or

  - Think about the model problem you can solve with the methods at hand.

Summary

- There are many reasons we want to consider using computational models to understand the Earth.
- The underlying equations for a minimum complexity problem are still challenging to solve numerically.
- Most geodynamic models employ a variant of the material point method.
- Major differences between packages occur in how the flow and energy problems are discretized.
- The two main approaches are Staggered-grid Finite Differences and the mixed Finite Element method.
- You will use both methods in your tutorials in the coming days.

Geodynamic Modelling Resources

- Gerya, T., 2019. *Introduction to numerical geodynamic modelling*. Cambridge University Press.
- Elman, H.C., Silvester, D.J. and Wathen, A.J., 2014. *Finite elements and fast iterative solvers: with applications in incompressible fluid dynamics*. Oxford university press.
- May, D. A., and Gerya, T. V. 2021. *Physics-based numerical modeling of geological processes*. In D. Alderton, & S. A. Elias (Eds.), Encyclopedia of geology (2nd ed., pp. 868–883). Acadamic Press, USA. https://doi.org/10.1016/b978-0-12-409548-9.12520-5
- May, D.A. and Knepley, M.G., 2023. *Numerical Modeling of Subduction. In Dynamics of Plate Tectonics and Mantle Convection* (pp. 539-571). Elsevier.
- van Zelst, I., Crameri, F., Pusok, A.E., Glerum, A., Dannberg, J. and Thieulot, C., 2021. *101 geodynamic modelling: How to design, carry out, and interpret numerical studies*. Solid Earth Discussions, 2021, pp.1-80.

Resources | Software

- A non-exhaustive list
- **Designed specifically for geodynamics**
    - https://github.com/UniMainzGeo/LaMEM
    - https://underworld2.readthedocs.io/en/v2.14.0b/
    - https://aspect.geodynamics.org/
- **General design, but used for geodynamics**
    - https://www.firedrakeproject.org/
    - https://fluidityproject.github.io/