PETSc Rocks

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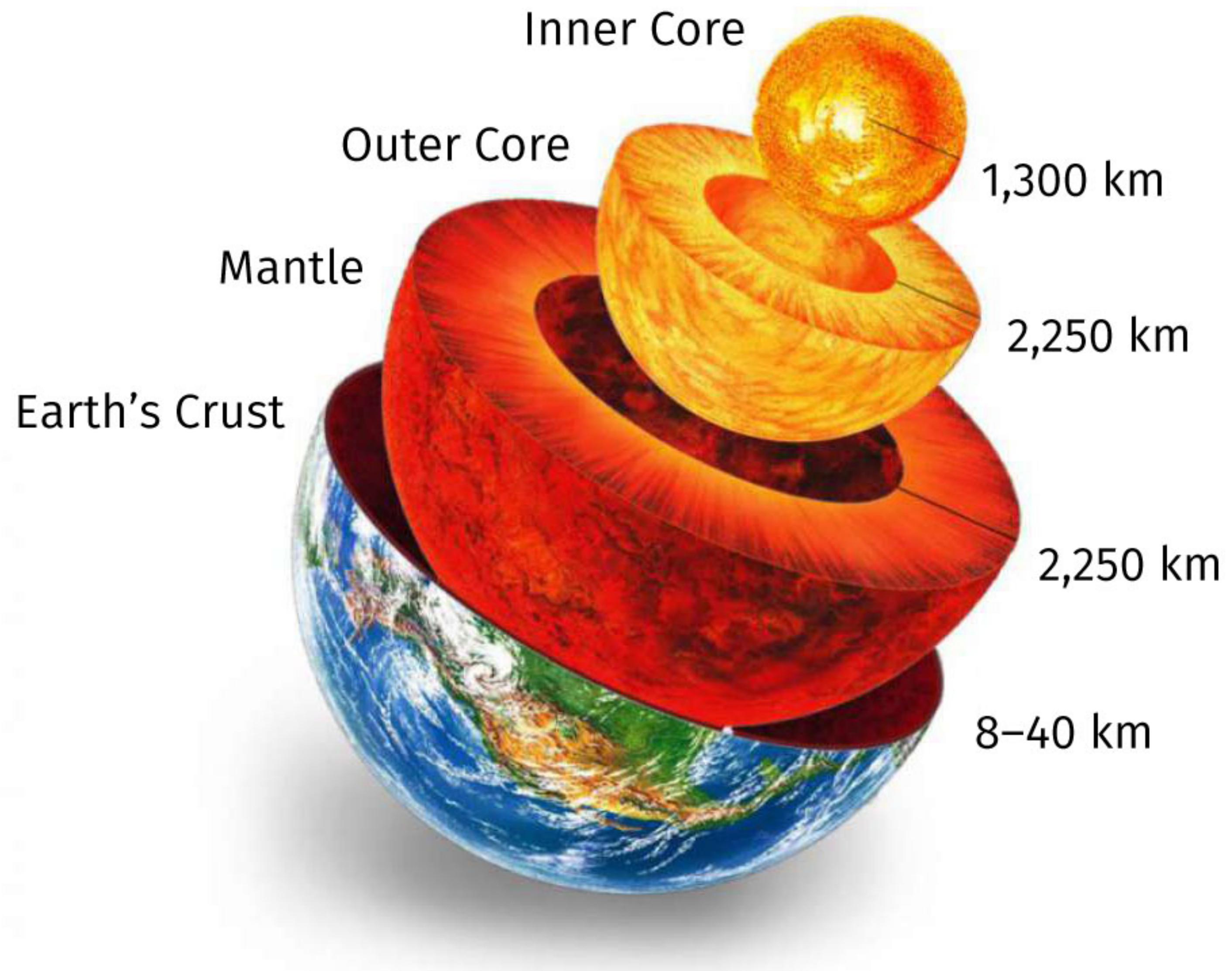
https://bitbucket.org/dmay | https://github.com/dmay23 | https://github.com/hpc4geo

Outline

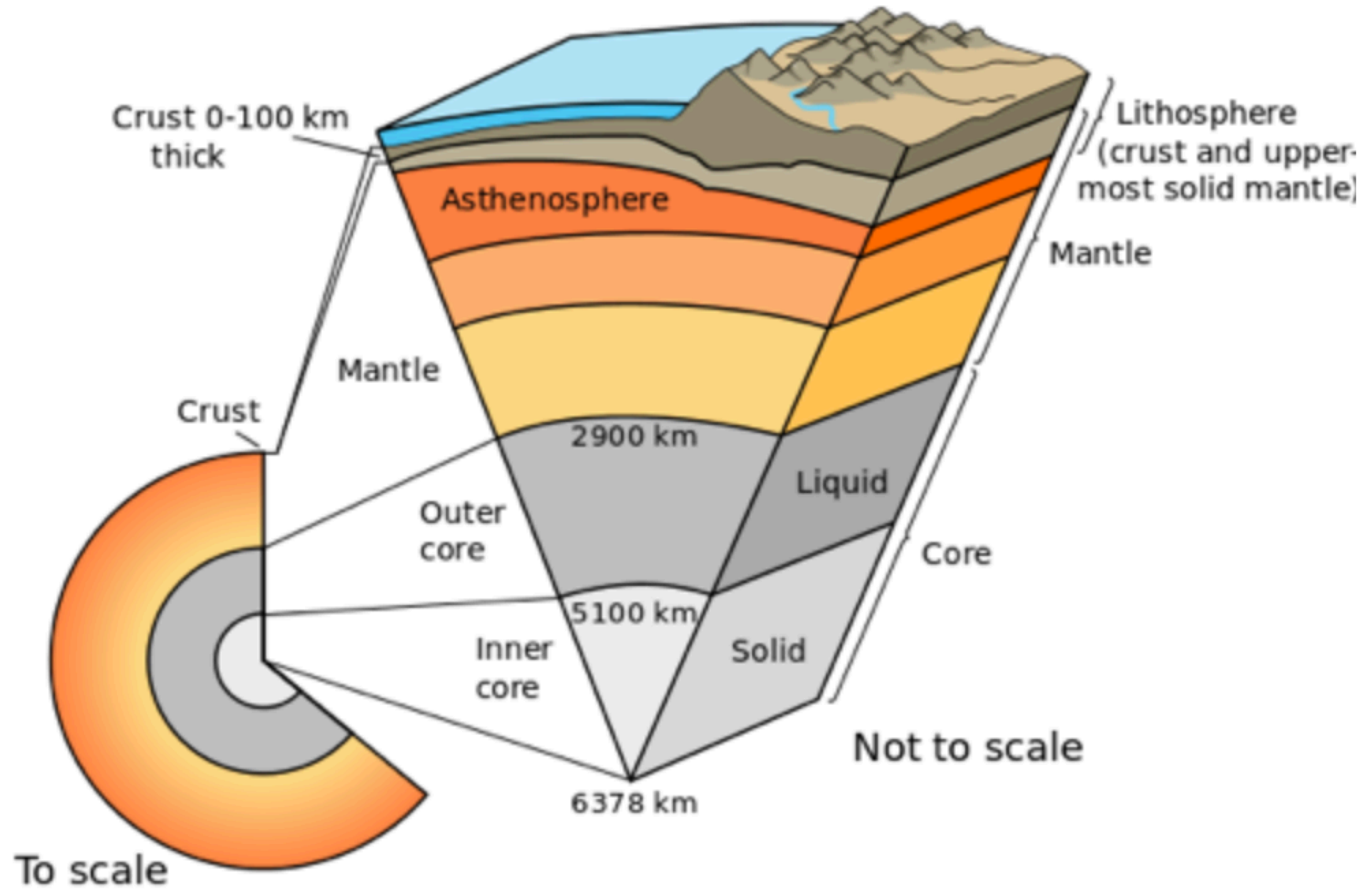
- The Earth, observations, and rheology of rocks
- Geodynamic modeling of long-time scale processes
- pTatin3D - a PETSc framework for regional scale geodynamics
- Application software driving PETSc dev
- Summary

Structure of the Earth

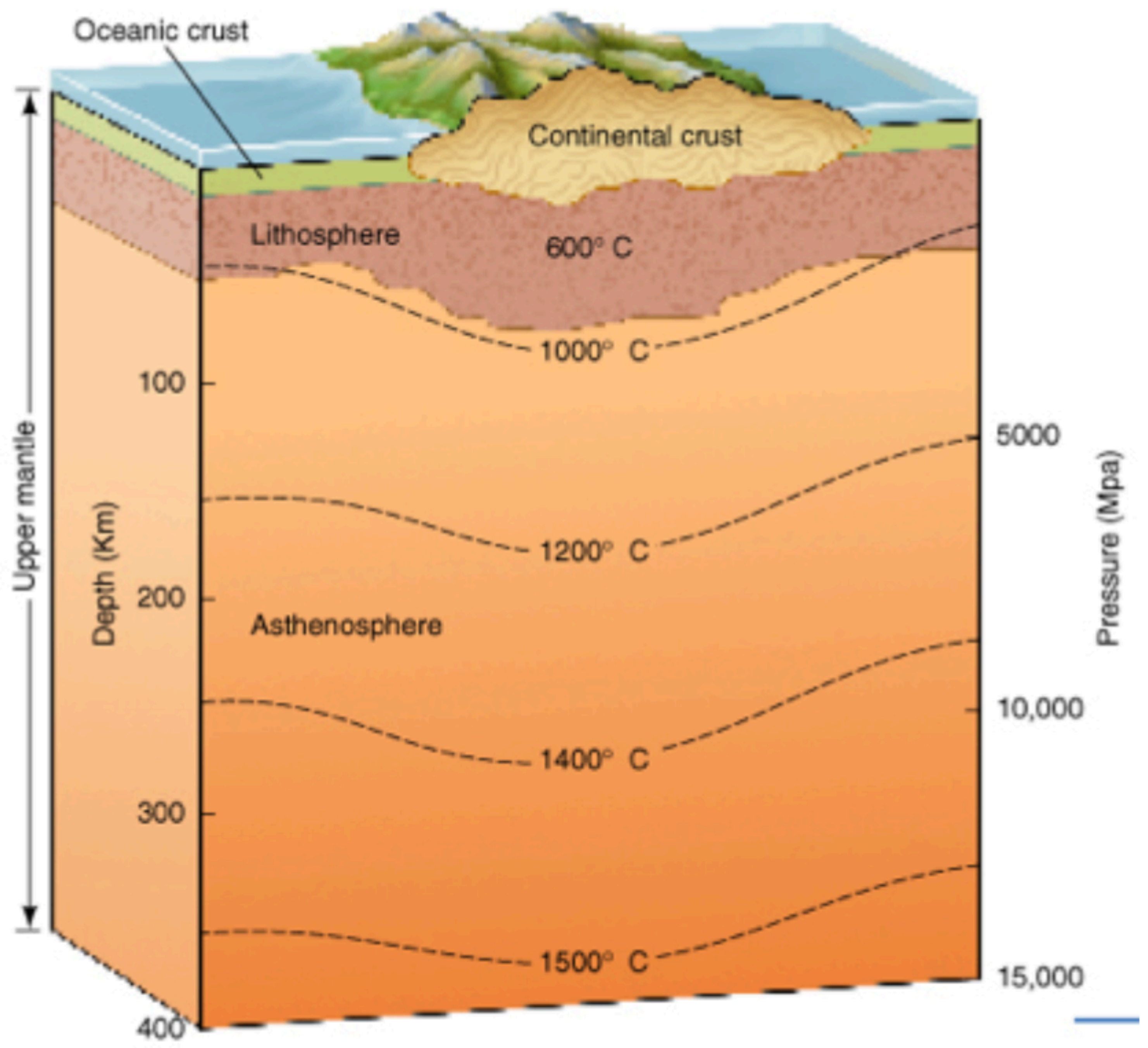
- The familiar onion model



https://www.the-dialogue.com/en/en66-how-plate-tectonics-is-connected-with-life-on-the-planet/



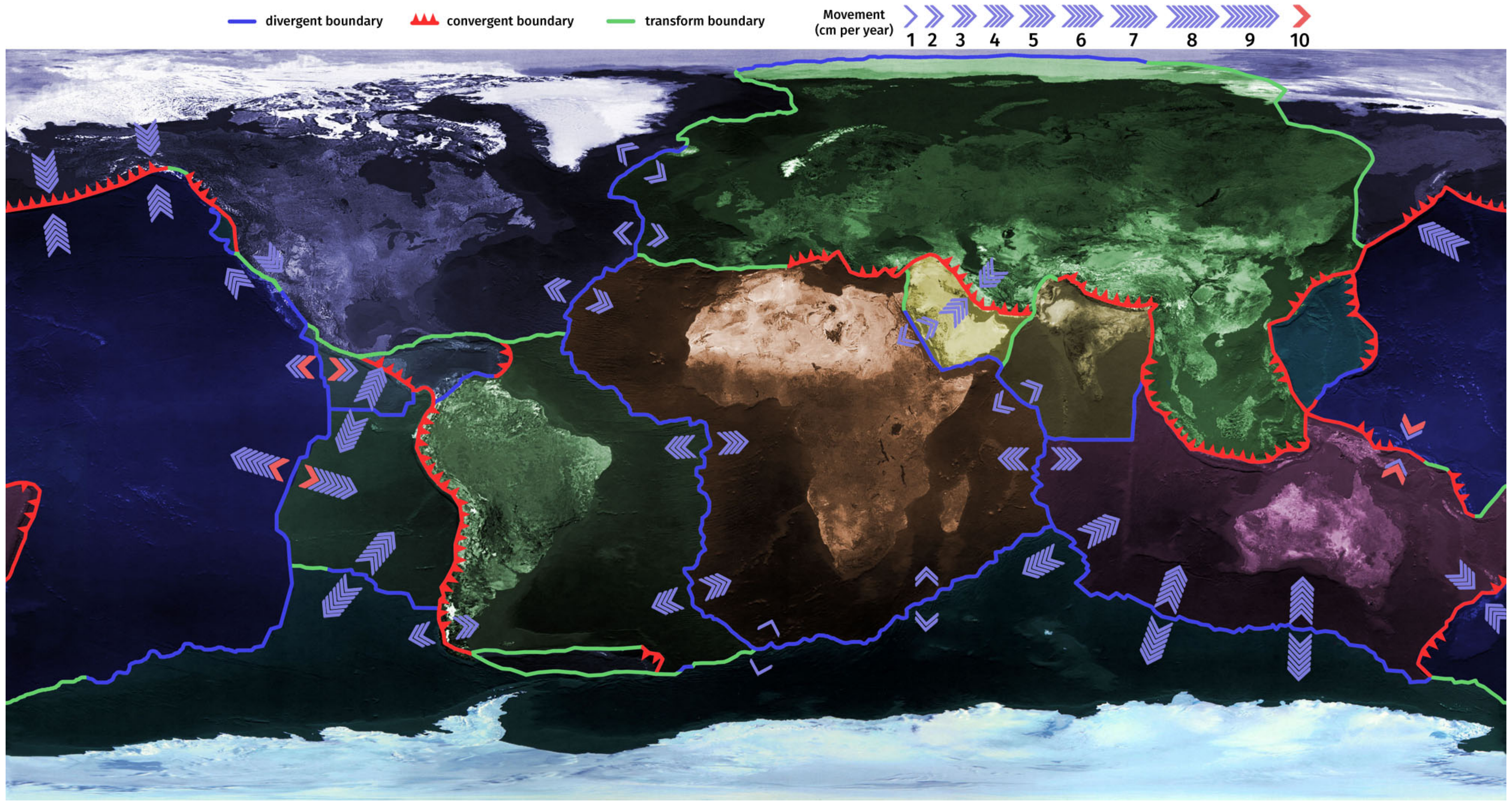
http://opengeology.org/textbook/2-plate-tectonics/



global scale **regional scale**

Plate tectonics paradigm

- A set of lithospheric plates covering the entire surface of the Earth. 7 major plates represent ~95% of the surface.
- Plates are composed of a mixture of different lithospheric materials, i.e. oceanic, continental.
- Plates
  - move (translate, rotate);
  - deform (primarily along their boundaries);
  - interact along their boundaries. Interactions depend on the boundary segment type.
- <u>The entire system is dynamic and time dependent.</u>
- The age of the tectonic style we observe today is highly debated, estimates range from 1B to 4B years old.



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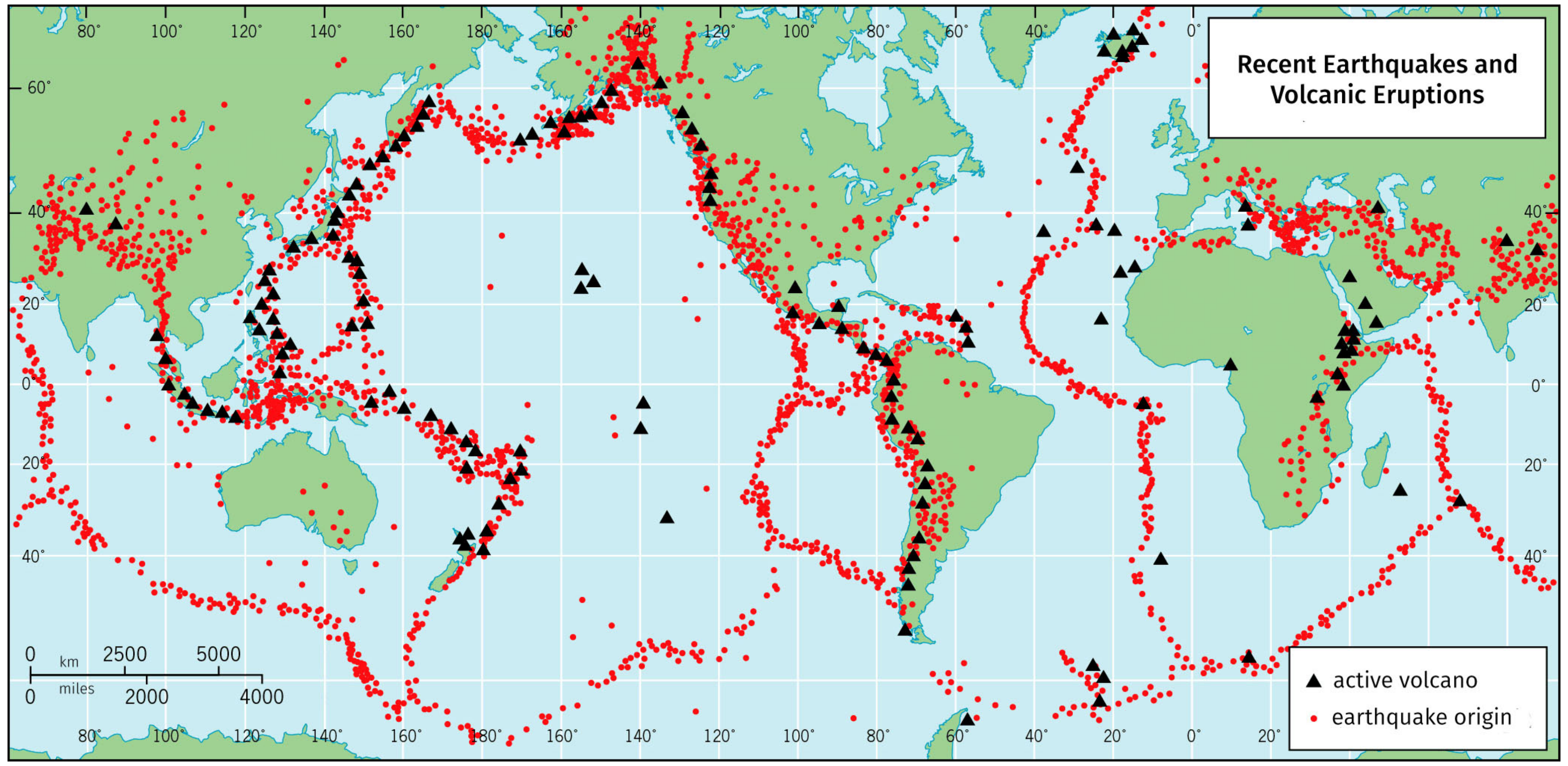
Earthquakes occur at plate boundaries

- Earthquakes (EQs) mainly concentrated along plate boundaries
- Other EQ related hazards include tsunamis



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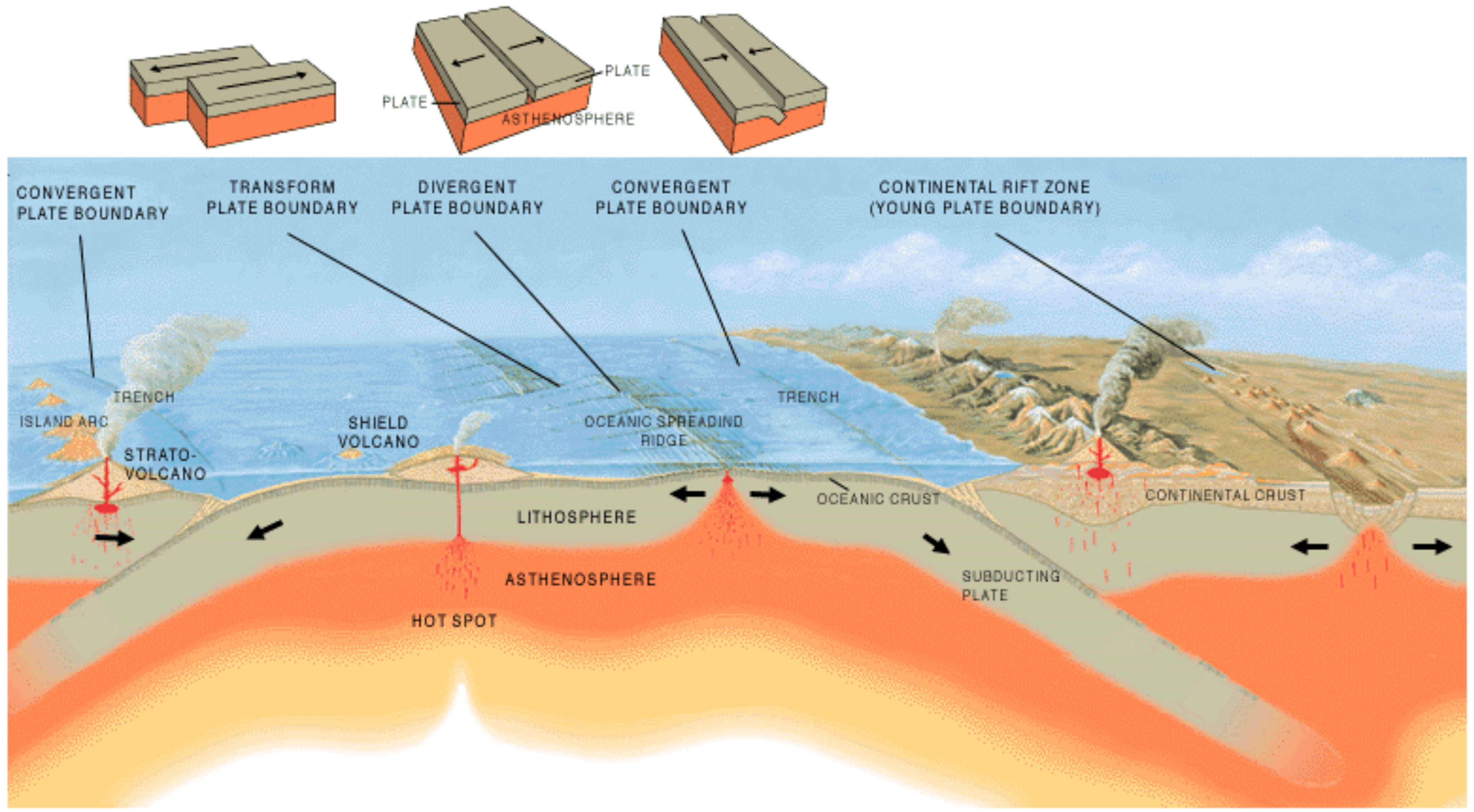
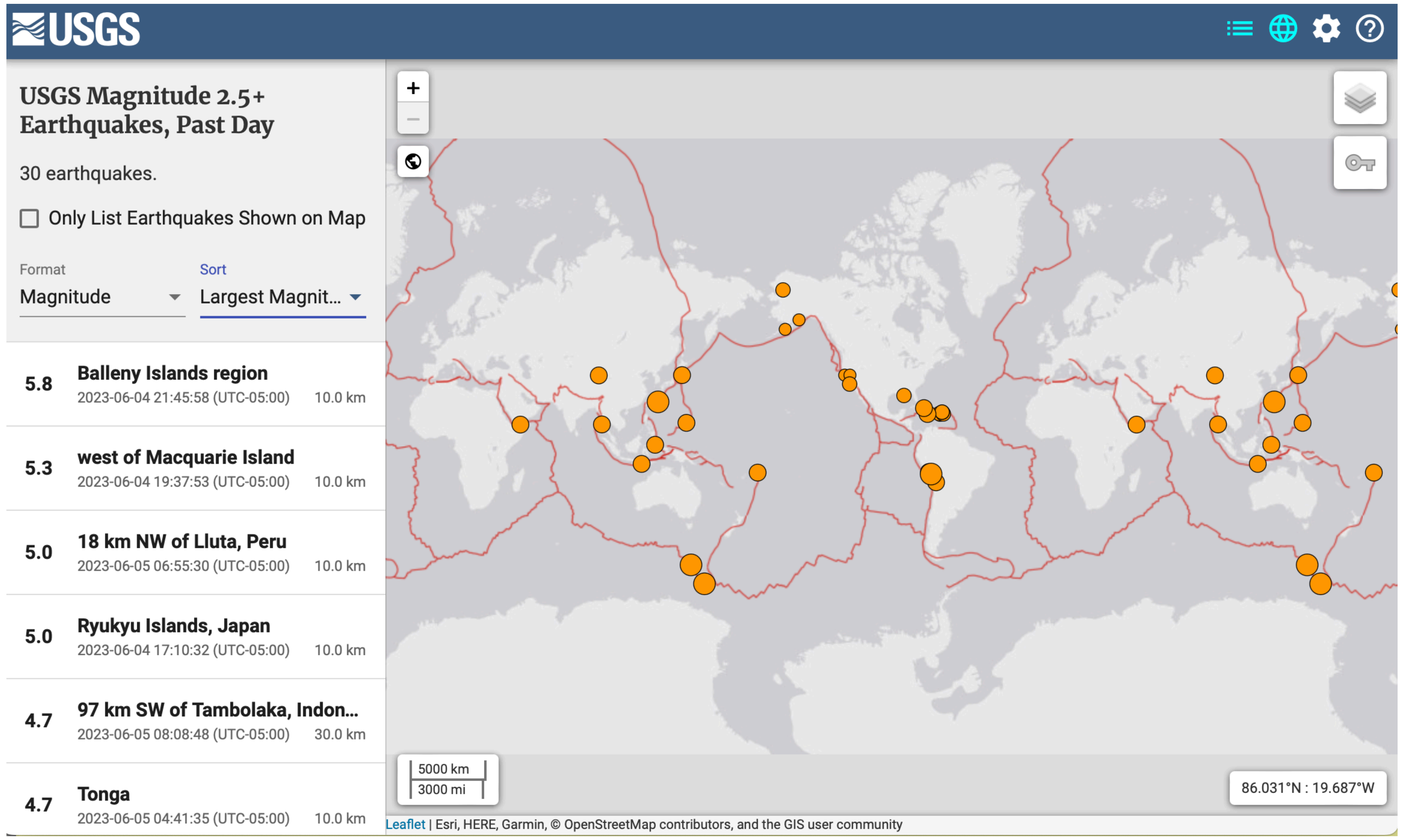
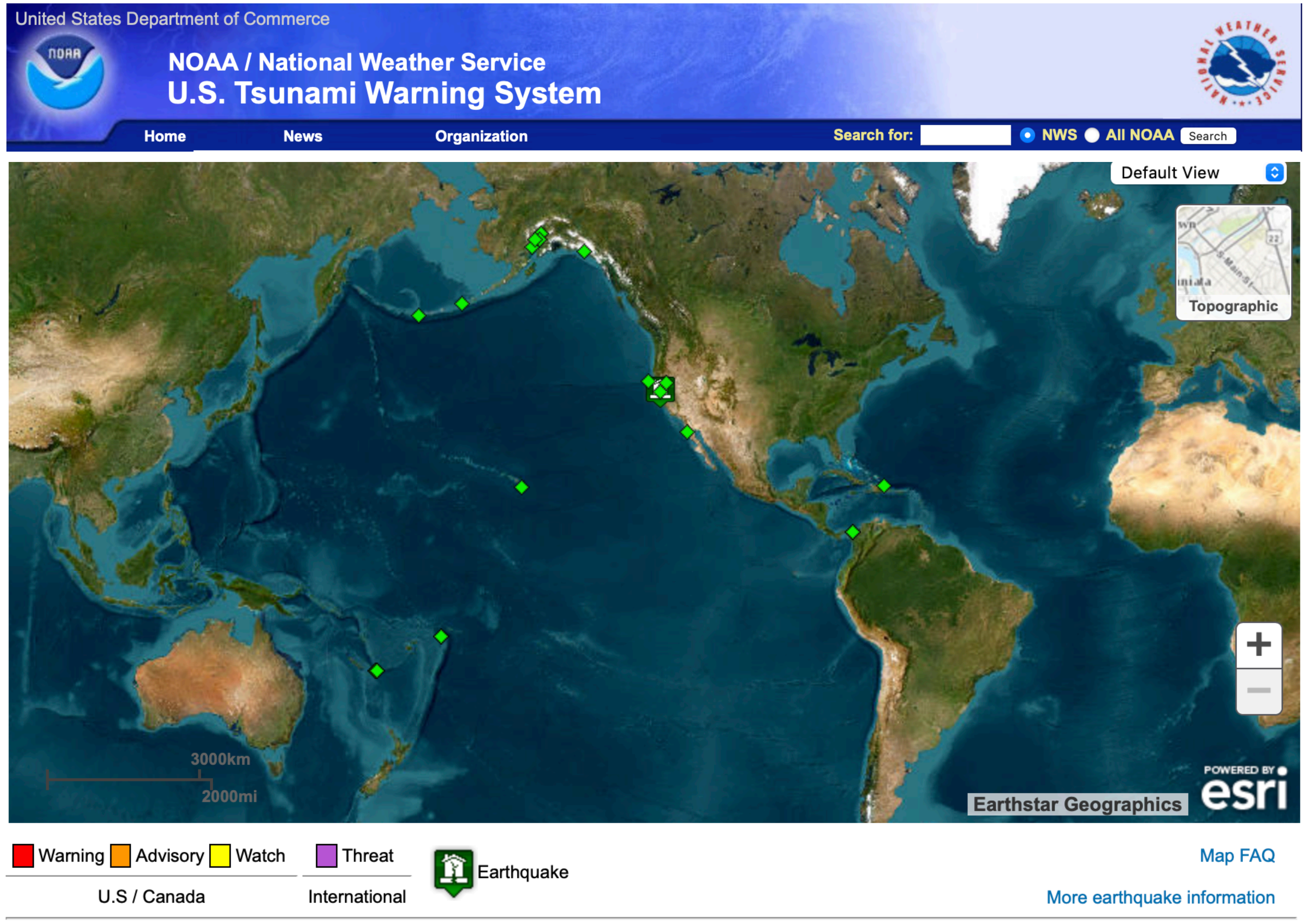


https://www.universetoday.com/43822/subduction-zone/

Seismic events happen all the time





Issued *	Origin Time *	Mag	Depth	Lat	Lon	Location	Messages	Additional Resources **
06-03-2023 12:06:19	06-03-2023 12:01:21	4.3	1 Mi.	38.7° N	122.7° W	65 MILES W OF SACRAMENTO, CALIFORNIA	AK/BC/US West Coast Informational #1	Select Resource
05-27-2023 16:53:51	05-27-2023 16:49:22	4.4	85 Mi.	60.3° N	152.9° W	70 MILES NW OF HOMER, ALASKA	AK/BC/US West Coast Informational #1	Select Resource
05-26-2023 02:20:50	05-26-2023 02:17:59	4.1	26 Mi.	61.7° N	150.9° W	50 MILES SW OF TALKEETNA, ALASKA	AK/BC/US West Coast Informational #1	Select Resource
05-25-2023 12:59:06	05-25-2023 12:54:33	4	7 Mi.	59.8° N	140.5° W	30 MILES NW OF YAKUTAT, ALASKA	AK/BC/US West Coast Informational #1	Select Resource

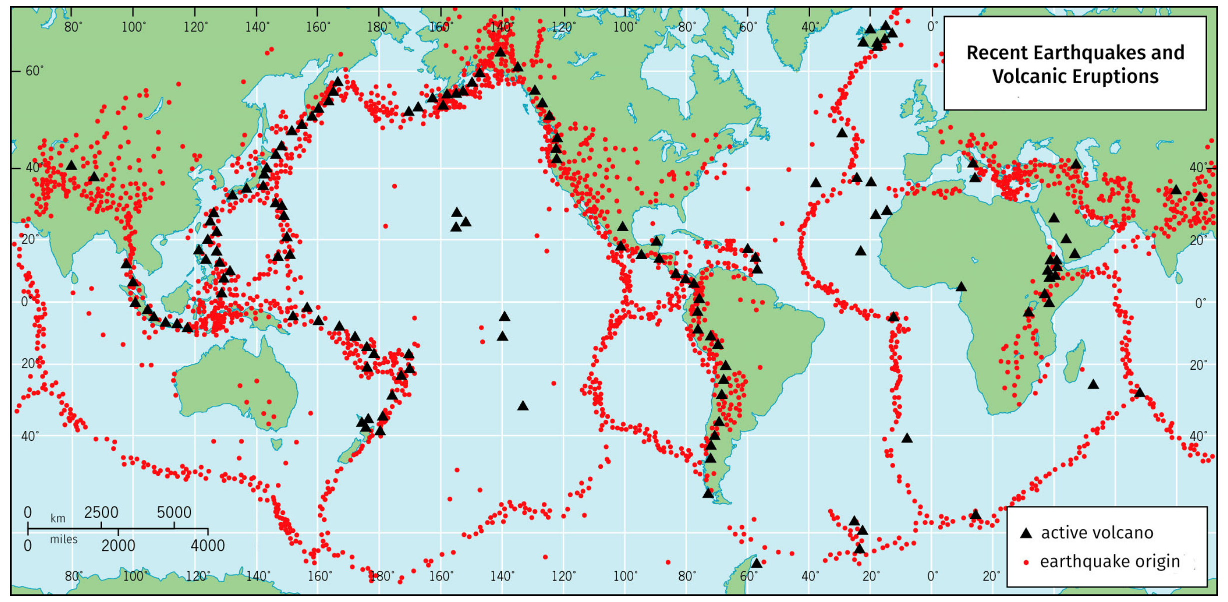
Rock rheology

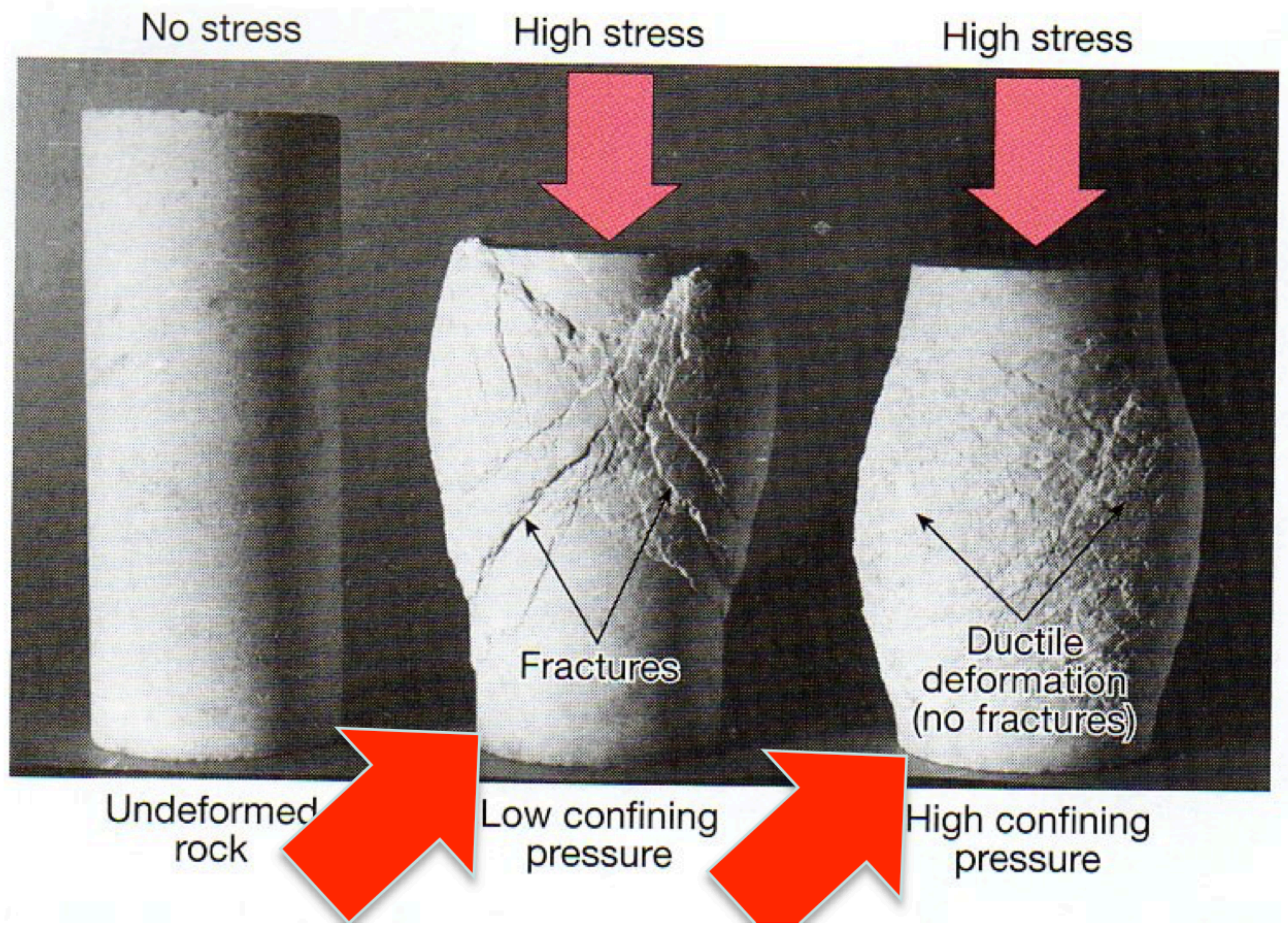
- Ductile and brittle

- Temperature dependent
- Strain-rate dependent
- Pressure dependent
- Path dependent

- Instability of rocks resulting from shear fracture, or unstable sliding at high pressure is the main cause of shallow source great earthquakes

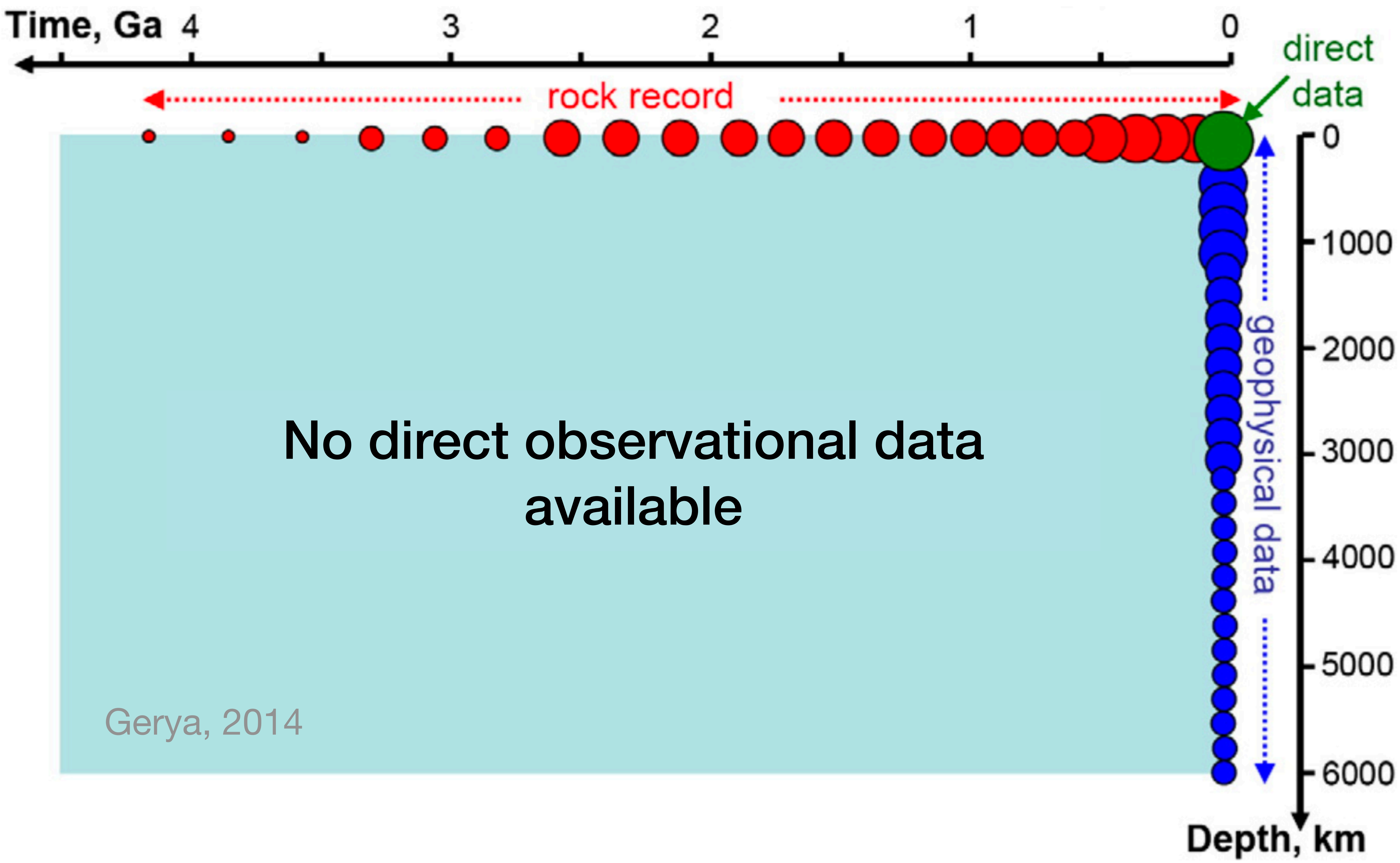
http://www.csun.edu/~dsw/lect8_geodyn_deform.pdf



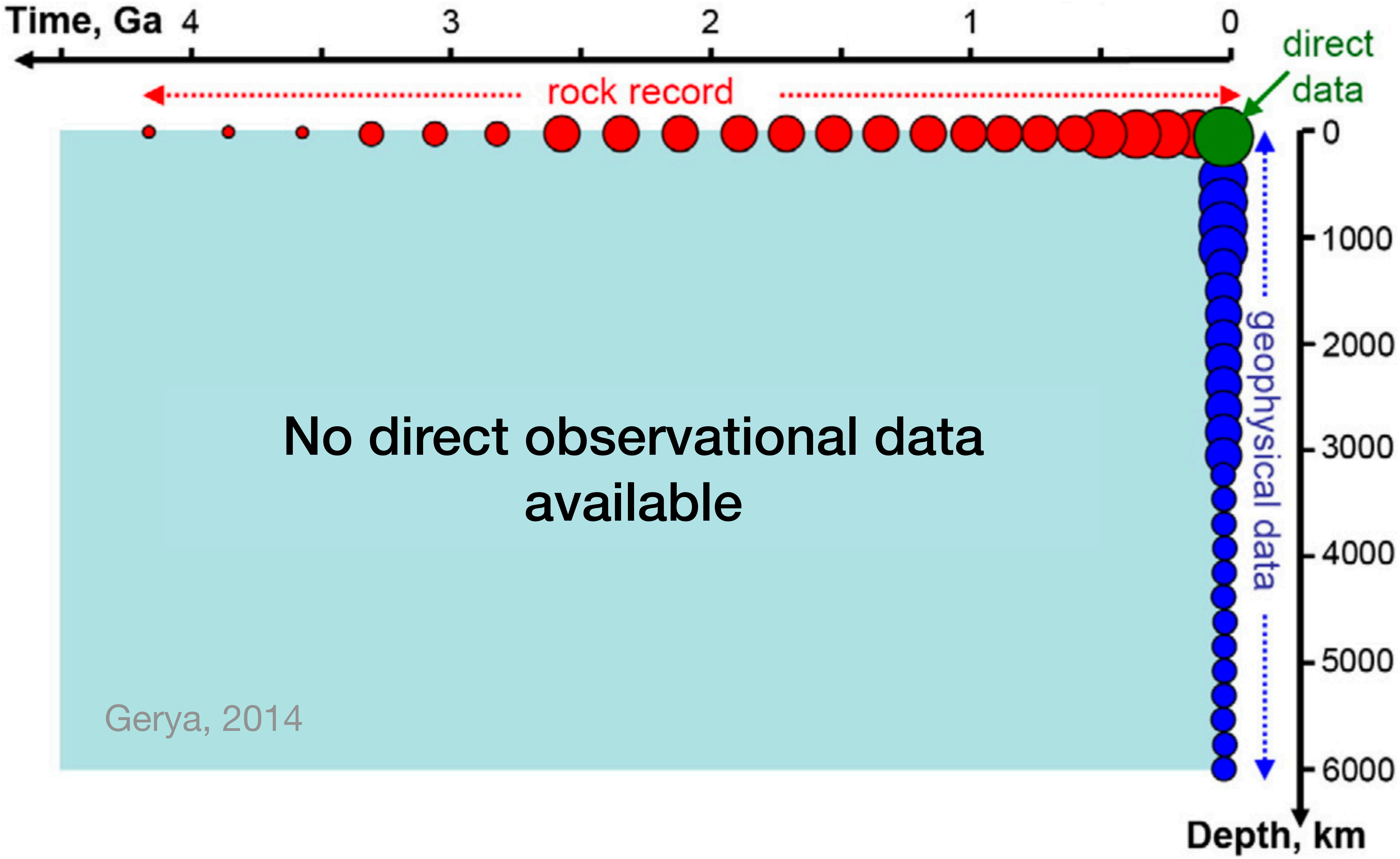


https://www3.nd.edu/~cneal/PlanetEarth/Chapt-11a-Rock-Mechanics.pdf

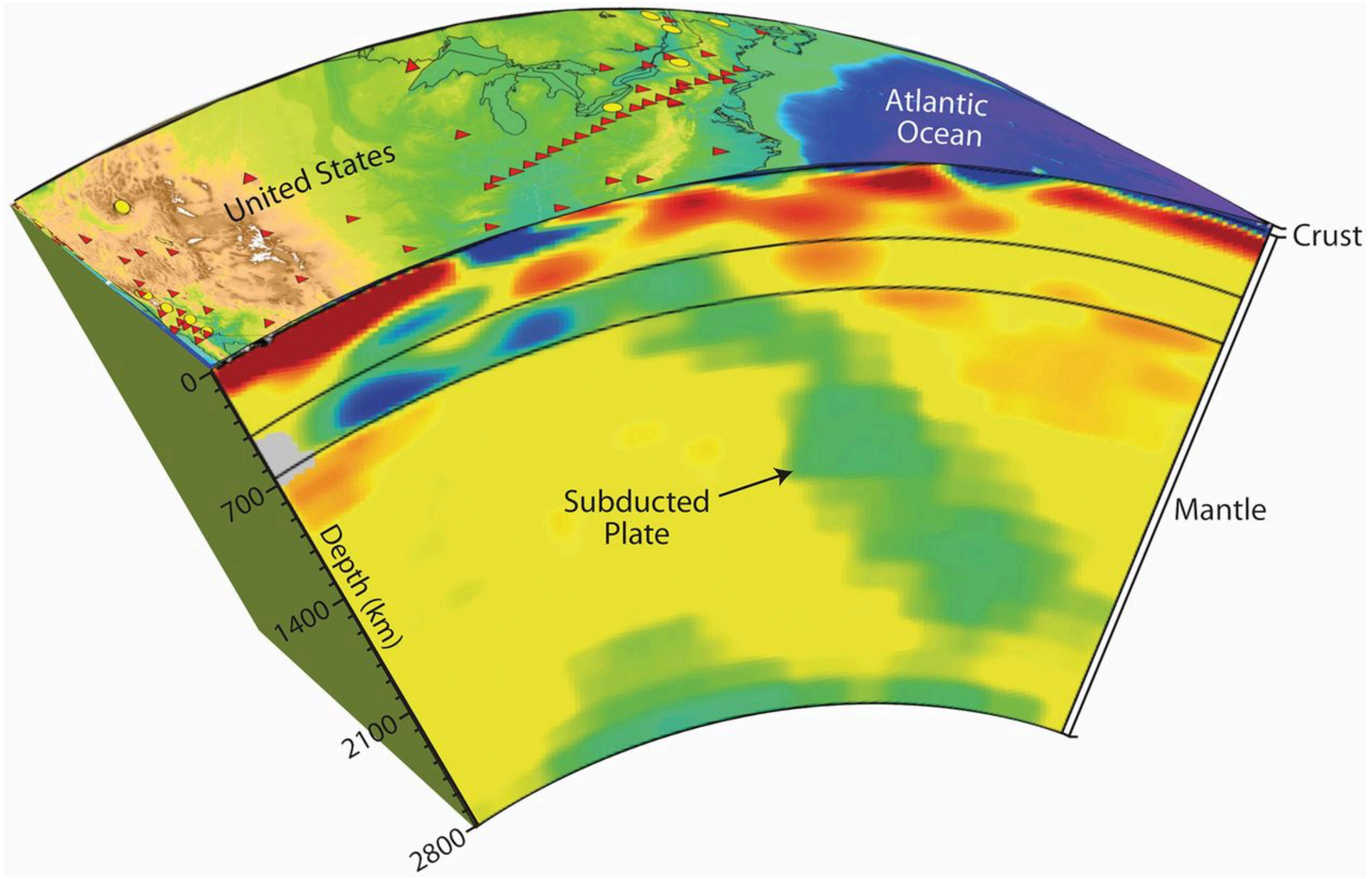
Locality of observational constraints



Geology



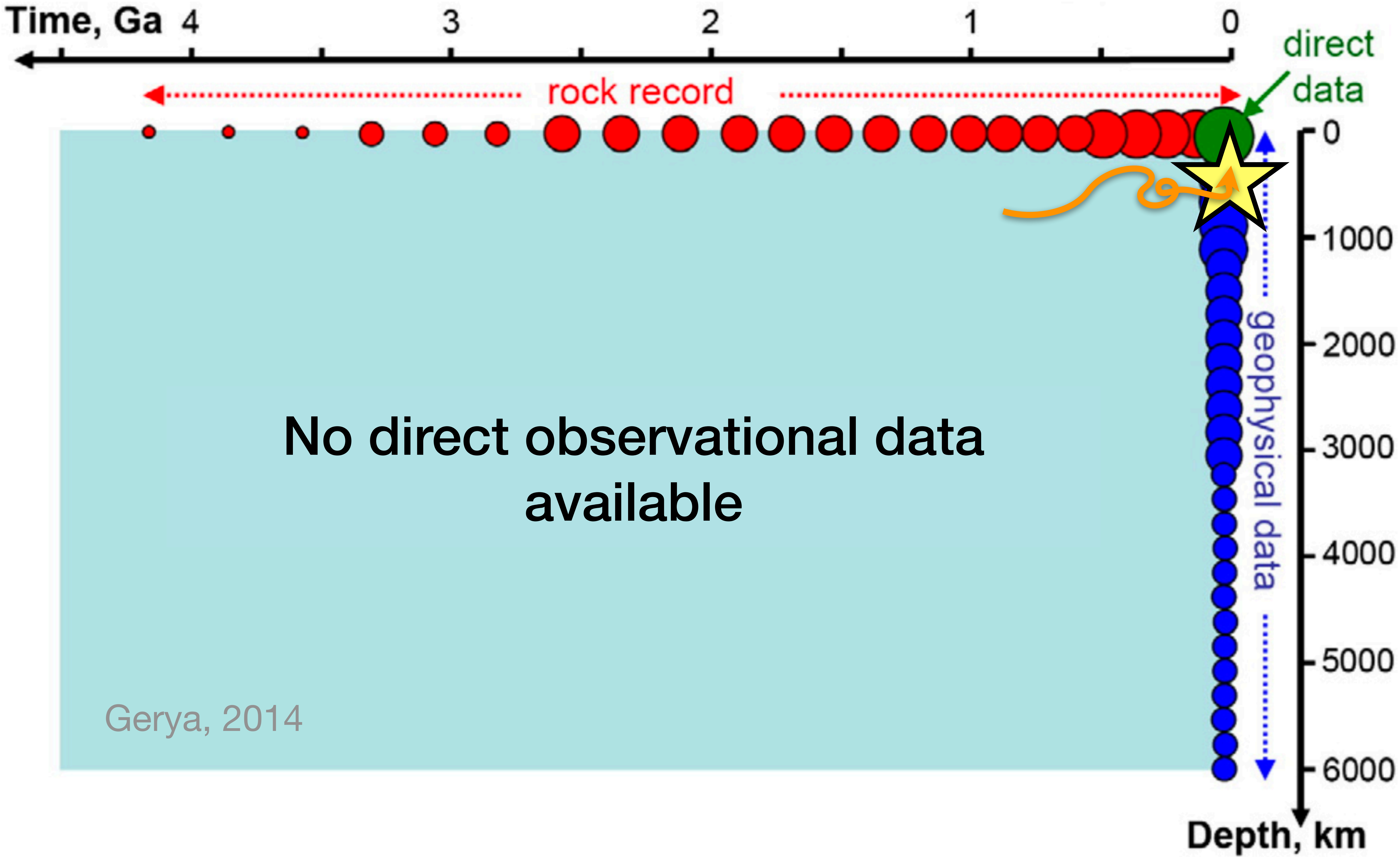
Geophysics



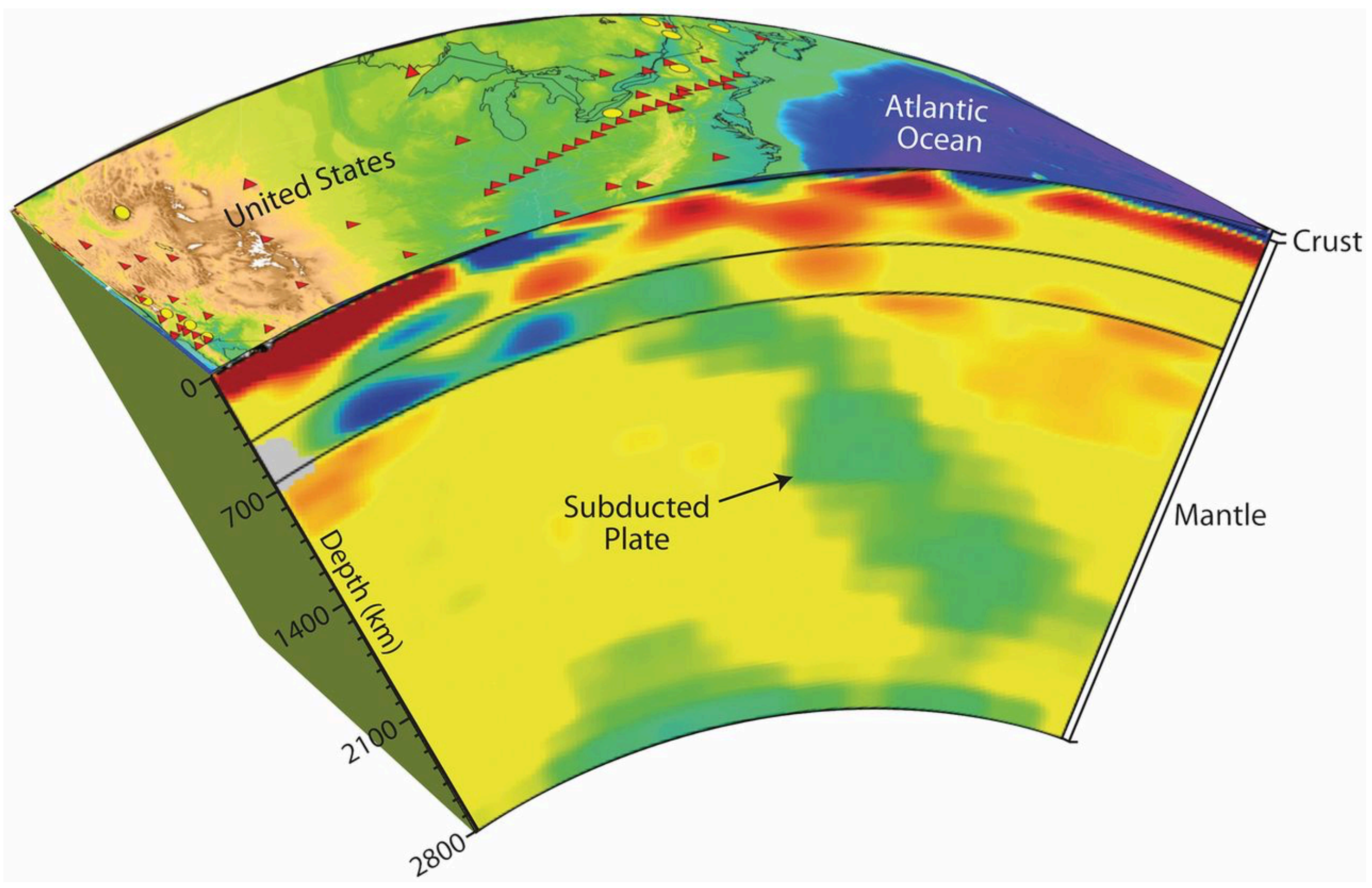
https://www.pnas.org/doi/10.1073/pnas.1909777116

Geology

- Physics-based hazard assessment is the way forward

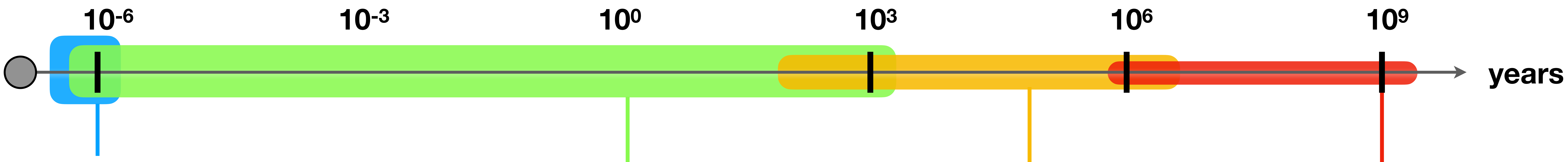


Geophysics

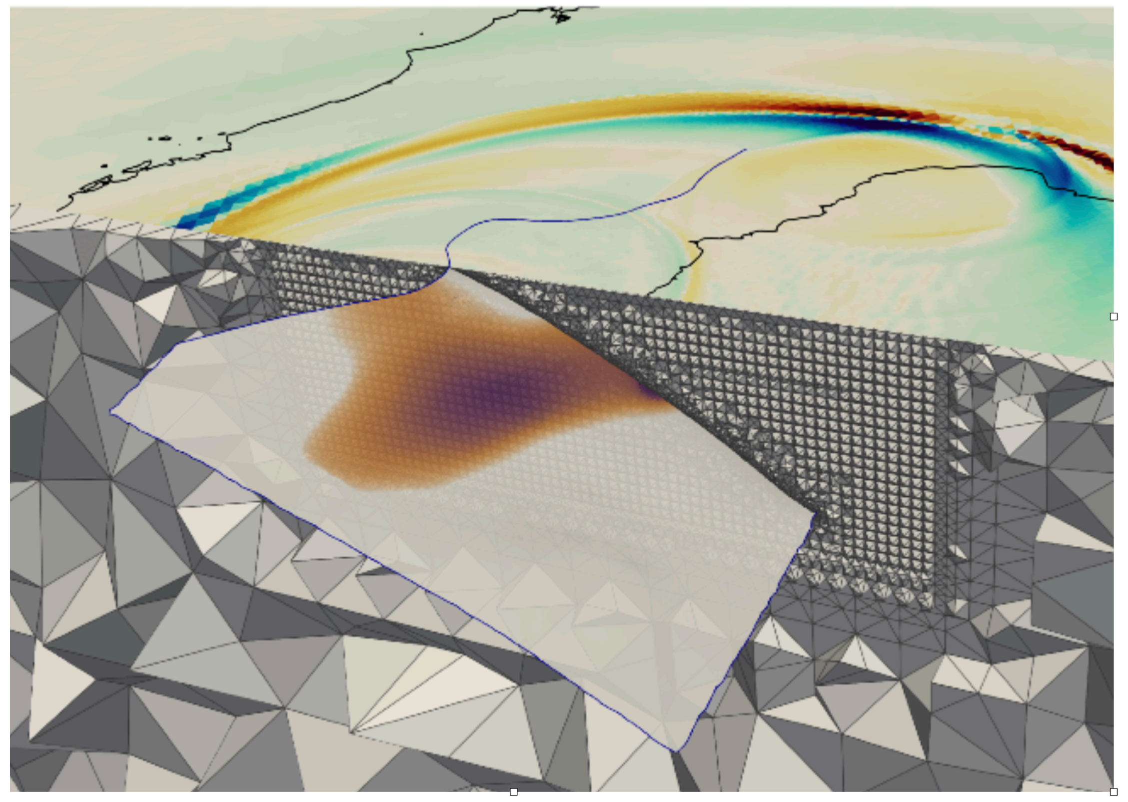


https://www.pnas.org/doi/10.1073/pnas.1909777116

Wide range of important time-scales

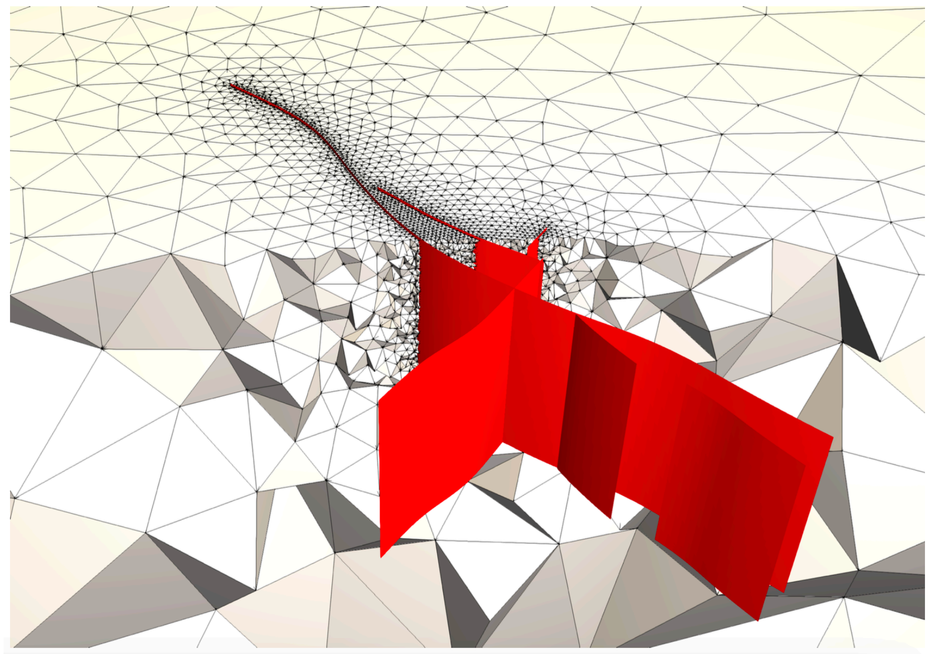


Wave propagation, dynamic rupture



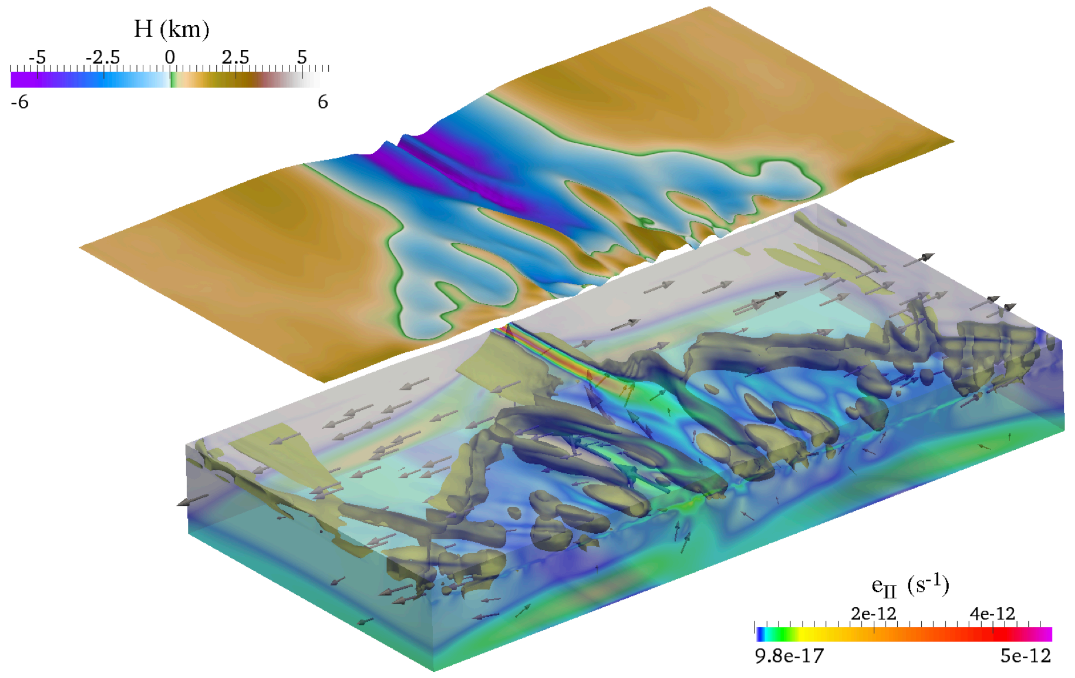
Biemiller, Gabriel, Ulrich (2022)

Seismic cycling



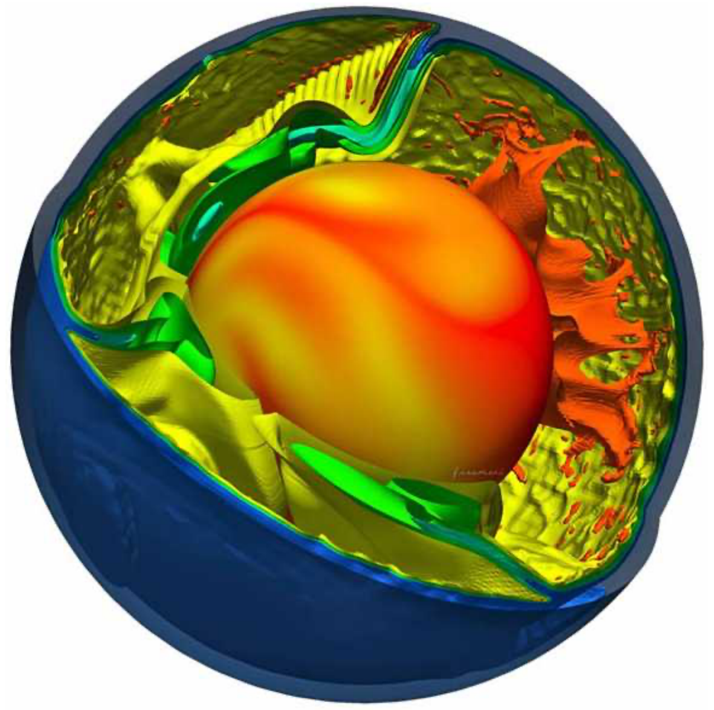
May, Uphoff, Gabriel (2022)

Regional geodynamics



May, Brown, le Pourhiet (2014)

Global geodynamics



F Crameri, P Tackley

- A spectrum of models for different time-scales

Modelling long-term dynamics

- Incompressible viscous flow
- Highly non-linear constitutive law
- Large deformation
- Large strain
- History dependent material behaviour
- Thermo-mechanical coupling
- Free-surface evolution
- 3D space + time

$$\frac{\partial \boldsymbol{\sigma}_{ij}}{\partial x_j} = \rho(T) g_i$$

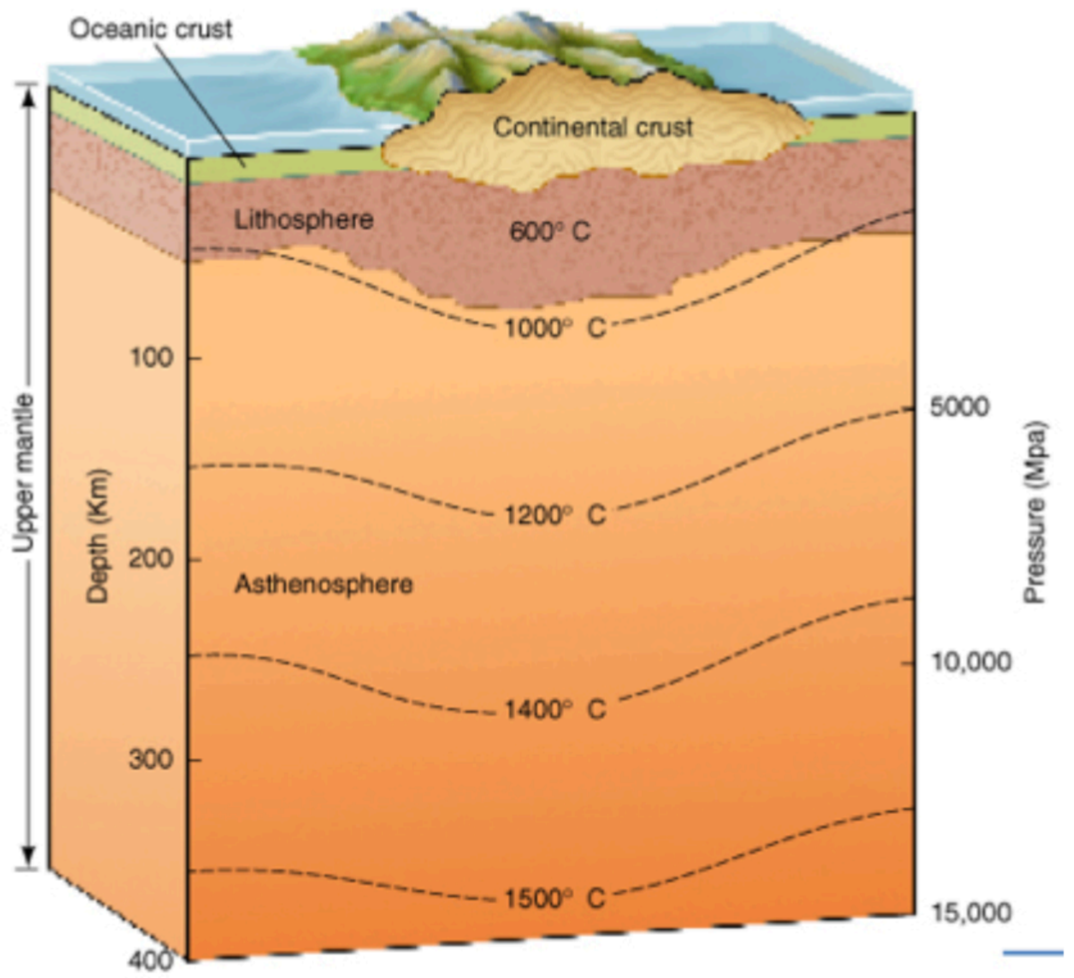
$$\frac{\partial \boldsymbol{V}_i}{\partial x_i} = 0$$

$$\rho C_p \frac{\mathrm{D}T}{\mathrm{D}t} = \frac{\partial}{\partial x_i}\left(k \frac{\partial T}{\partial x_i}\right) + \rho H$$

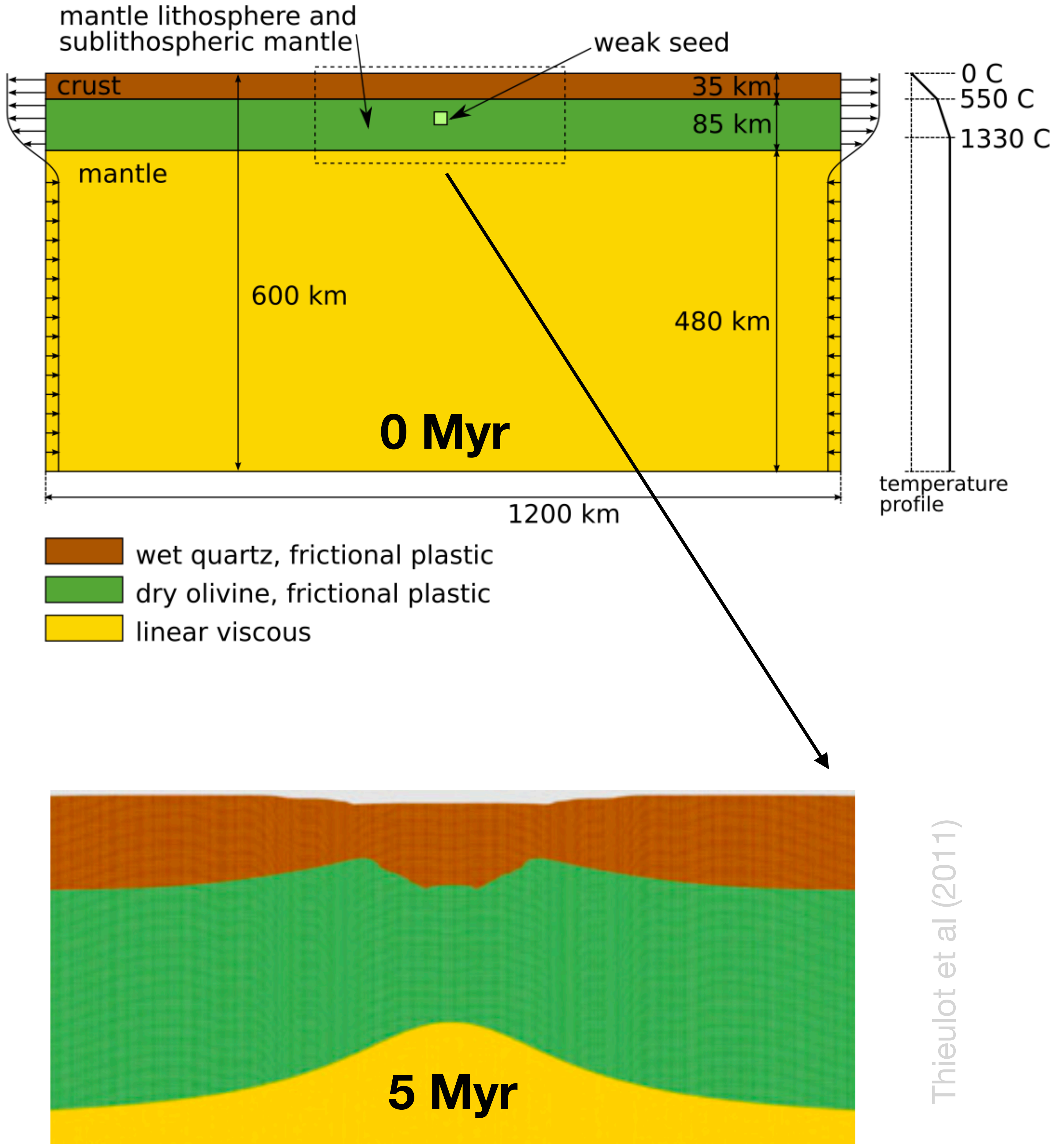
$$D_{ij} = D_{ij}^{\mathrm{e}} + D_{ij}^{\mathrm{v}} = \frac{\overset{\triangledown}{\boldsymbol{\tau}}_{ij}}{2\mu} + \frac{\boldsymbol{\tau}_{ij}}{2\eta}$$

$$|\boldsymbol{\tau}| < \boldsymbol{\tau}_{\mathrm{yield}} = \tan\varphi P + C$$

Modelling long-term dynamics

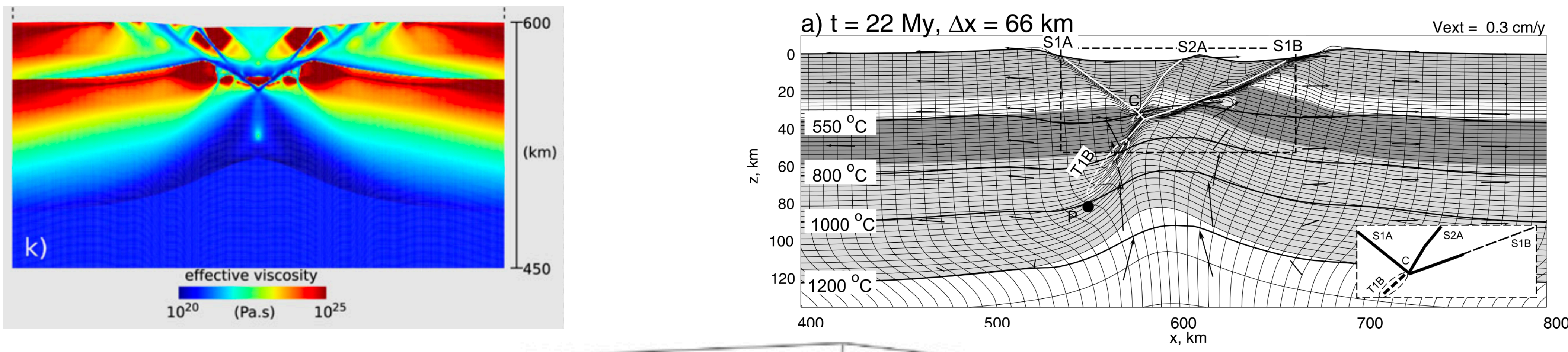


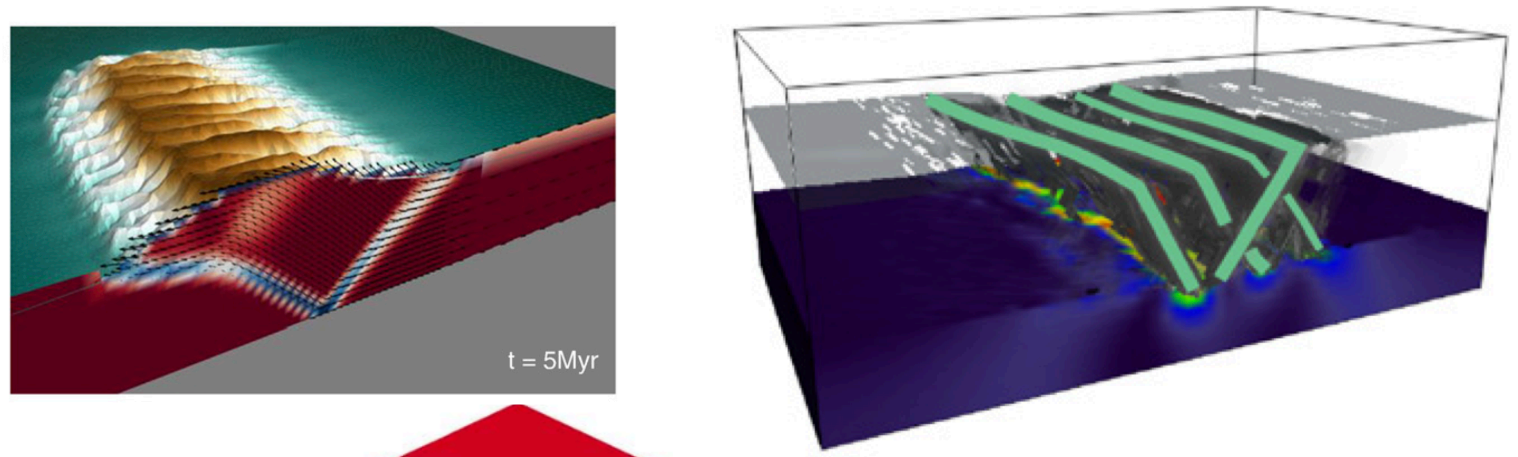
- **Large deformation**
- **Large strain**
- **History dependent material behaviour**
  - Use material points —> Lagrangian particles
  - Particles advected through mesh
  - Material point properties projected onto mesh



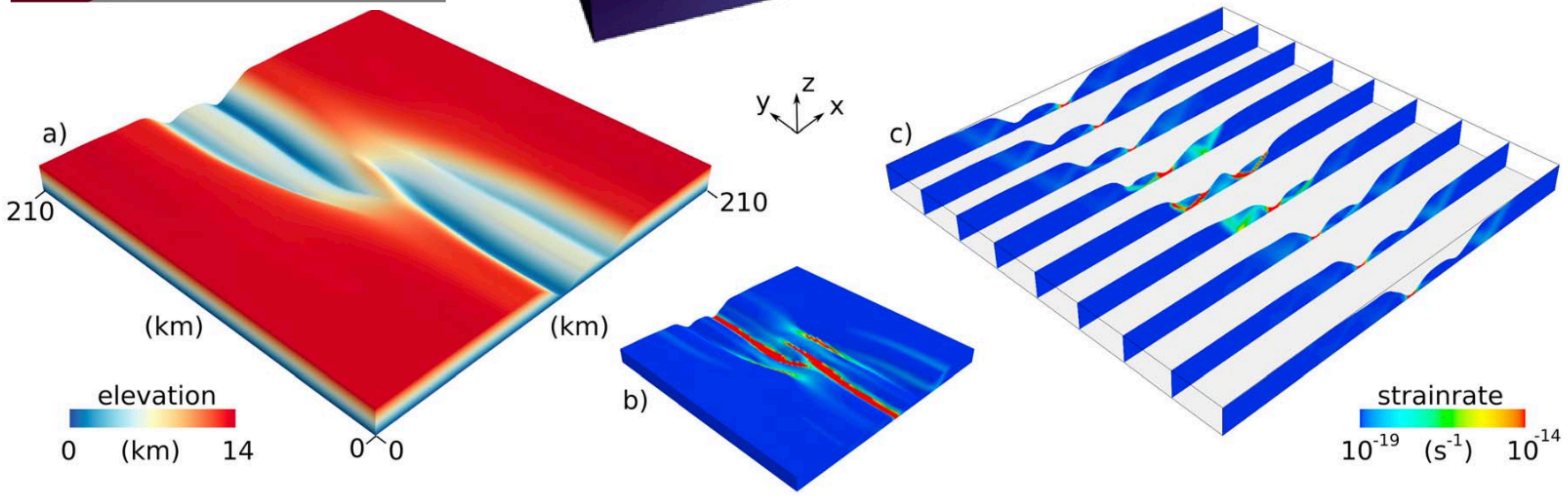
Thieulot et al (2011)

Modelling progress over the years

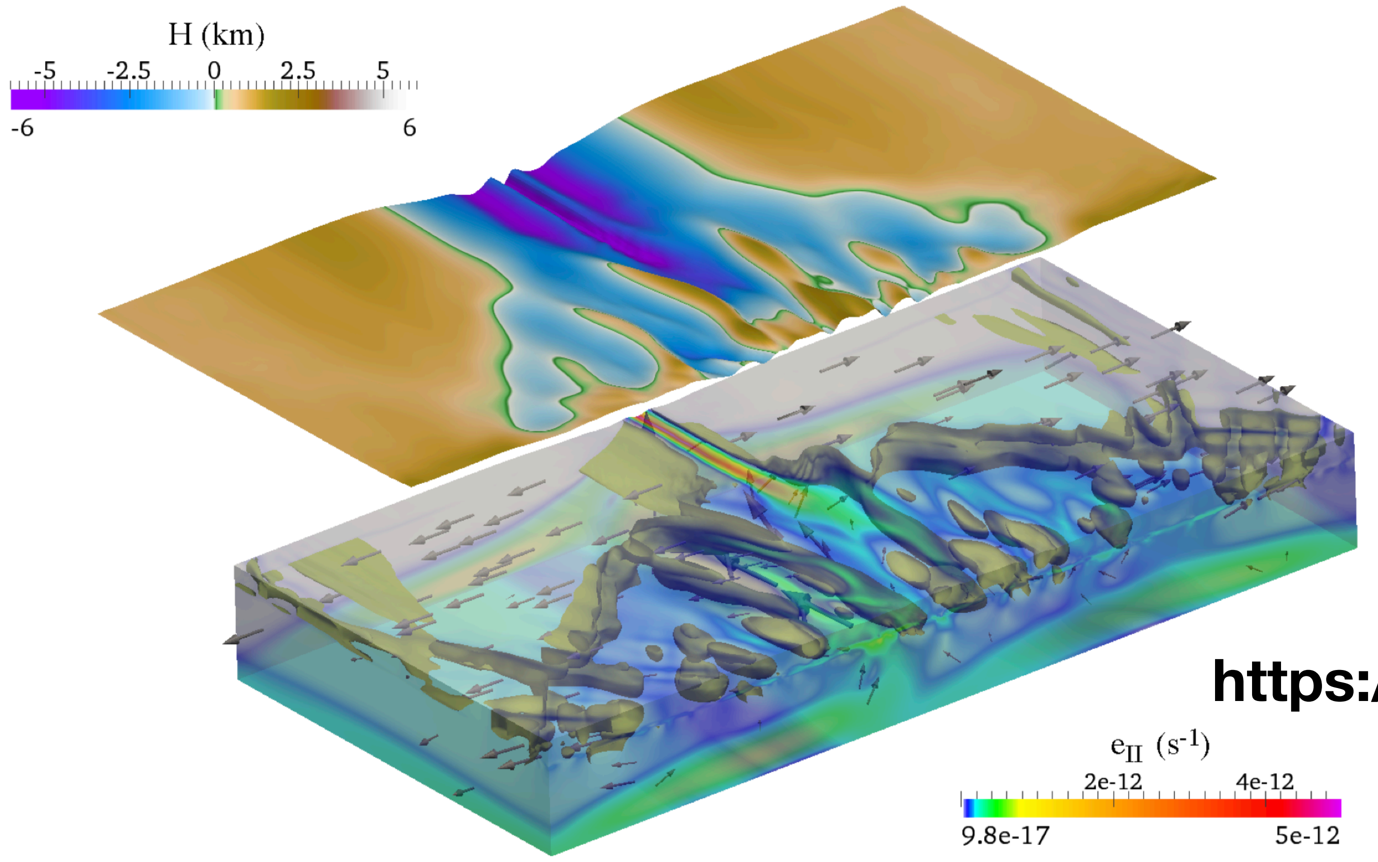




Huismans et al (2003)
Moresi et al (2007)
Braun et al (2008)
Thieulot et al (2011)
Allken et al (2012)

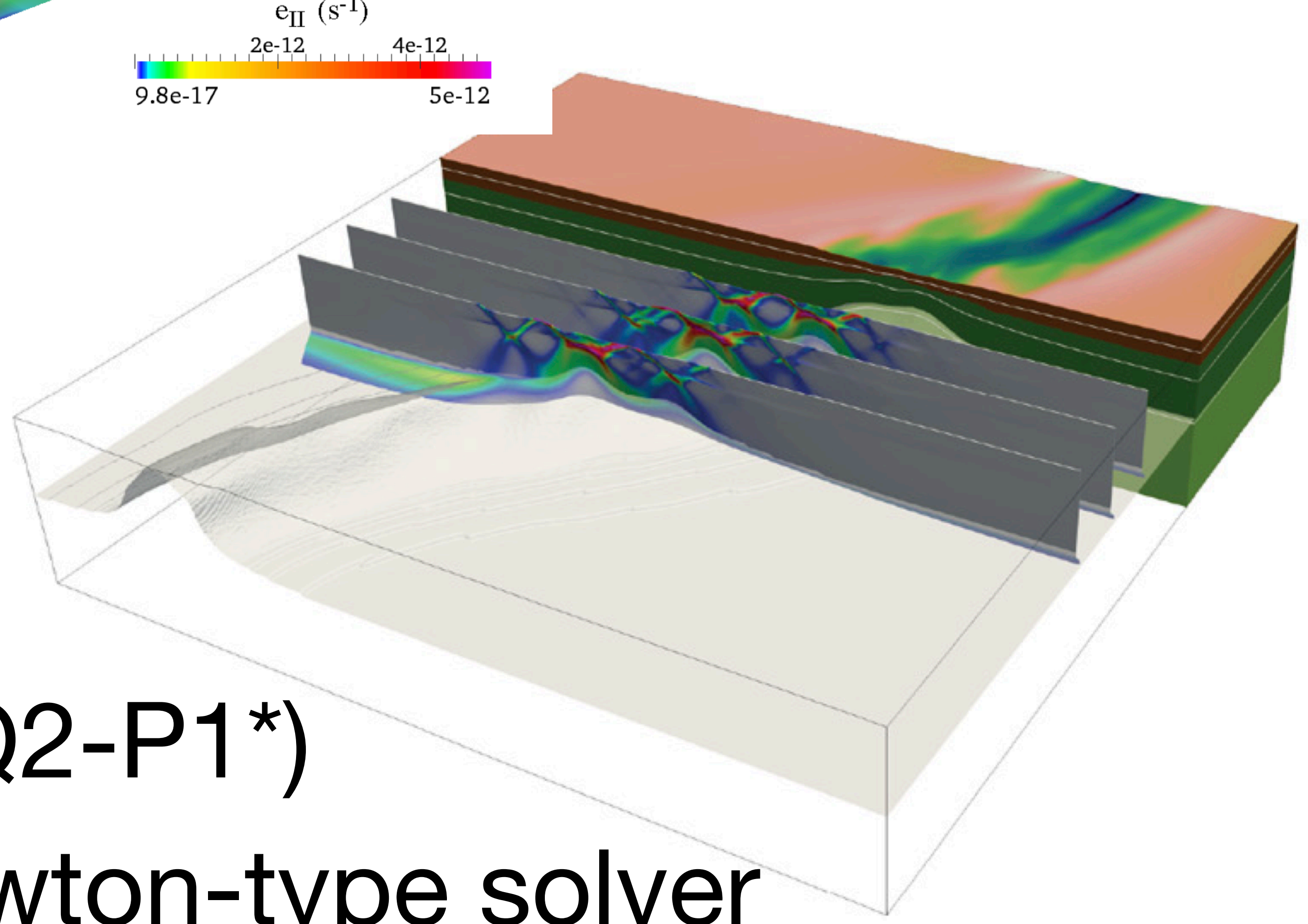


- Non inf-sup stable disc. (Q1-P0)
- Penalty method or SCR
- Sparse direct (threaded, MPI), multigrid
- Non-scalable
- 2D high res. or 3D low res.



pTatin3D

https://bitbucket.org/ptatin/ptatin3d



May et al (2014, 2015)
Le Pourhiet et al (2018)
Duclaux et al (2020)
Jourdon (2020)
Wolf et al (2022)

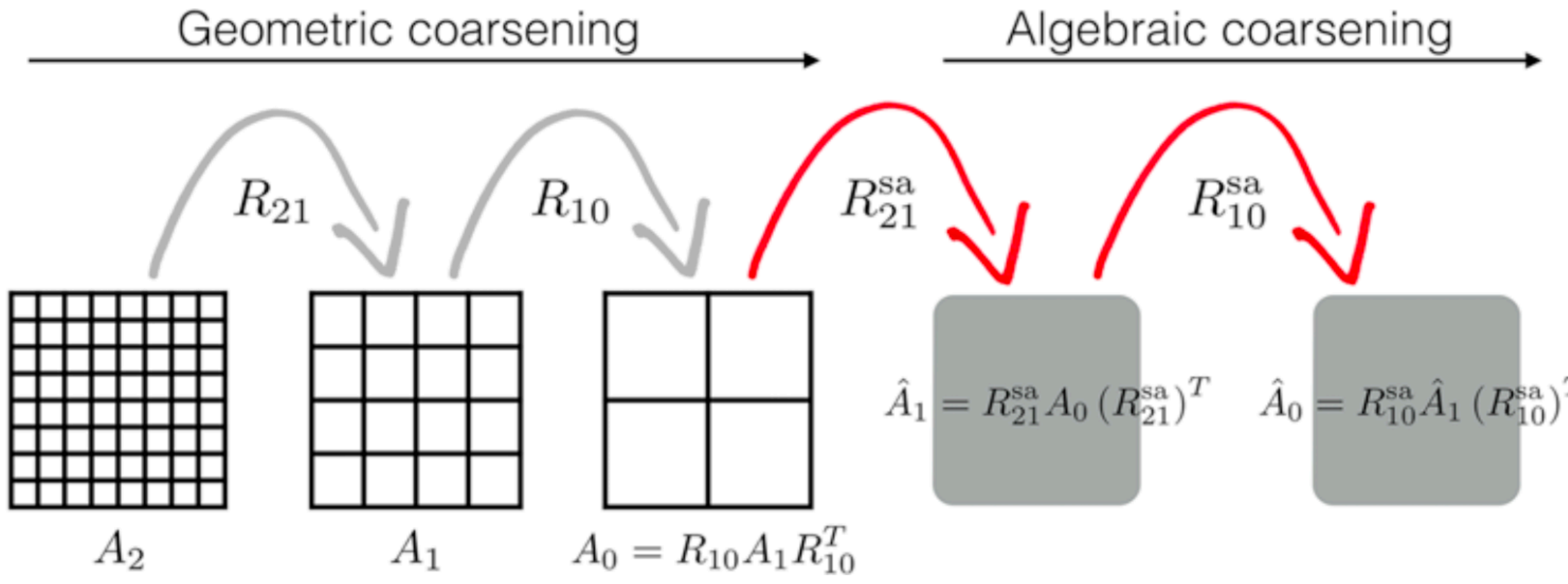
- Stable disc. (Q2-P1*)
- Full space Newton-type solver
- Distributed memory
- Hybrid multigrid
- Scalable
- 3D high resolution

pTatin3D | Designed for scalability and efficiency

- Structured mesh (`DMDA`) with Q2-P1* discretization
- Newton Krylov framework (`SNES`)
- Iterate on the velocity-pressure system | `MatNest`, `PCFieldsplit` preconditioner
- Assembled (AS) or matrix-free (MF) operators
  - Naive, tensor, tensor+AVX, CUDA, …
- Run-time multigrid customization
  - Level-wise grid coarsening
  - Selection of coarse grid operator construction and matrix type
    - e.g. re-disc MF, re-disc AS., Galerkin, MF Galerkin
  - Repartitioning of coarse grids onto fewer MPI ranks

$$\mathbf{J}\delta\mathbf{X} = -\mathbf{F} \rightarrow \begin{bmatrix} \mathbf{J}_{uu} & \mathbf{J}_{up} \\ \mathbf{J}_{pu} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \delta\mathbf{u} \\ \delta\mathbf{p} \end{bmatrix} = -\begin{bmatrix} \mathbf{F}_u \\ \mathbf{F}_p \end{bmatrix}$$

$$\mathbf{B}_U = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{0} & -\mathbf{S} \end{bmatrix}$$



pTatin3D | Design

- **Flexible solver configurable**
    - `PCFieldsplit` matrix-free

$$\mathbf{J}\delta\mathbf{X} = -\mathbf{F} \rightarrow \begin{bmatrix} \mathbf{J}_{uu} & \mathbf{J}_{up} \\ \mathbf{J}_{pu} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \delta\mathbf{u} \\ \delta\mathbf{p} \end{bmatrix} = - \begin{bmatrix} \mathbf{F}_u \\ \mathbf{F}_p \end{bmatrix}$$

        - Schur complement reduction or full-space
        - Upper, lower factorizations
        - Exact or inexact J_{uu} solve
    - Matrix type flexibility (Native PETSc `MATAIJ` or `MatShell`)
    - Portable Extensible Toolkit for Solver Composition

pTatin3D | Design

- **Minimize memory footprint and maintain robustness**
  - `MatNest` —> avoid the copy with `PCFieldsplit`

$$\mathbf{B}_U = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{0} & -\mathbf{S} \end{bmatrix}$$

  - Matrix-free kernels via `MatShell`
  - Chebyshev as a smoother
  - `KSPGCR` —> flexible Krylov method, residual access for free
- **High resolution simulations (large MPI comm. size)**
  - Pipelined Krylov methods
  - Multigrid on structured grids require repartitioning `PCTelescope`

pTatin3D | Design

- **History variables discretized via a set of Lagrangian particles**
  - Dedicated object to handle
    - arbitrary data types associated with a particle
    - dynamic sizing / re-sizing of the #particles per MPI rank
  - Dedicated object to handle communication arbitrary particle data
  - This became `DMSwarm`.

Moving your app. code —> PETSc

- **Discuss your ideas with the developers to**
  - assess feasibility
  - Determine necessary generalizations, abstractions required
  - `PCTelescope` and `DMSwarm` required many discussions
- **Benefits**
  - Unload the maintenance burden
  - Reduce the size of your own code base
  - Share your work with others
  - Work with a great project and great people
  - Become a developer one day

PETSc Rocks

- Is both a statement of what I model using PETSc, and how great PETSc is.

- My software and research would <u>not</u> be possible with PETSc
- My reasons
  - runtime configuration
  - library wide component inter-operability
  - adoption and integration of new contributions from users
  - my CS and math skills improved working with PETSc and its developers
  - <u>development team support</u>