Genesis, Preservation and Destruction of Mantle Heterogeneity

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Michael Manga's 2012 lecture
Louise Kellogg's 2014 lecture

Two papers on Lagrangian Coherent Structures

Peacock and Haller, Physics Today, 2013
Haller, ARFM, 2015

http://shaddenlab.berkeley.edu/uploads/LCS-tutorial/overview.html

Reading Material

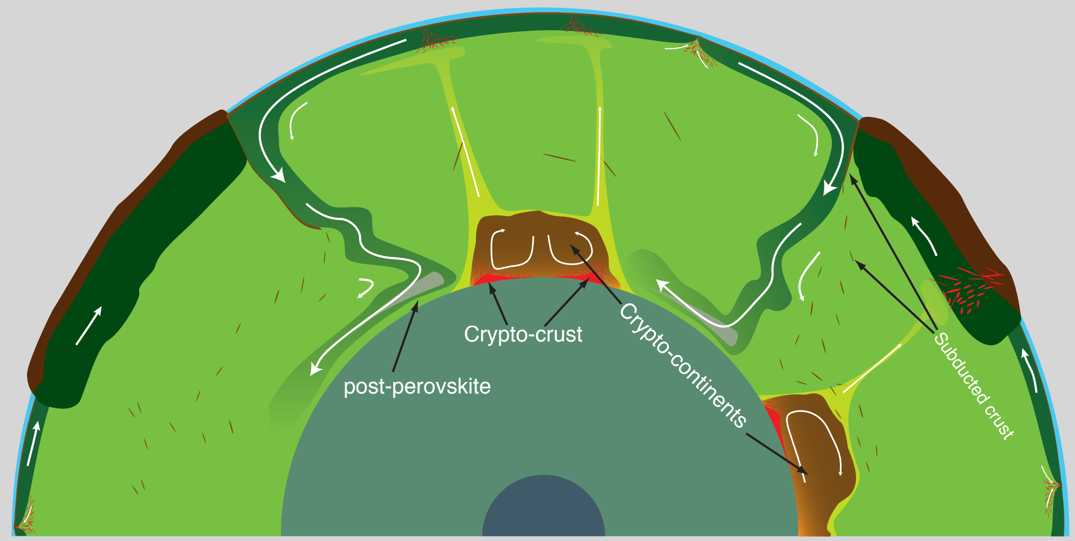
Origin
- Primordial
- Convective/Tectonic Processes

Location of Heterogeneity
- Where is the Physical Reservoir- Source region
- Length-scales
  - What controls it?

Preservation, Destruction and Time Scales
- Stirring and mixing processes
- Controlled by mantle dynamics, material properties and Earth's history

What do we see seismically/geochemically?
- Major element- seismically detectable, "easy" physical location, tied to genesis
- Minor element- possibly seismic correlation (e.g. Dalton et al., 20xx)
- Trace-only identifiable geochemically tied to:
  - genesis
  - source region vs entrained material
  - processes in melting region
  - sampling

Creation, Destruction, Survival



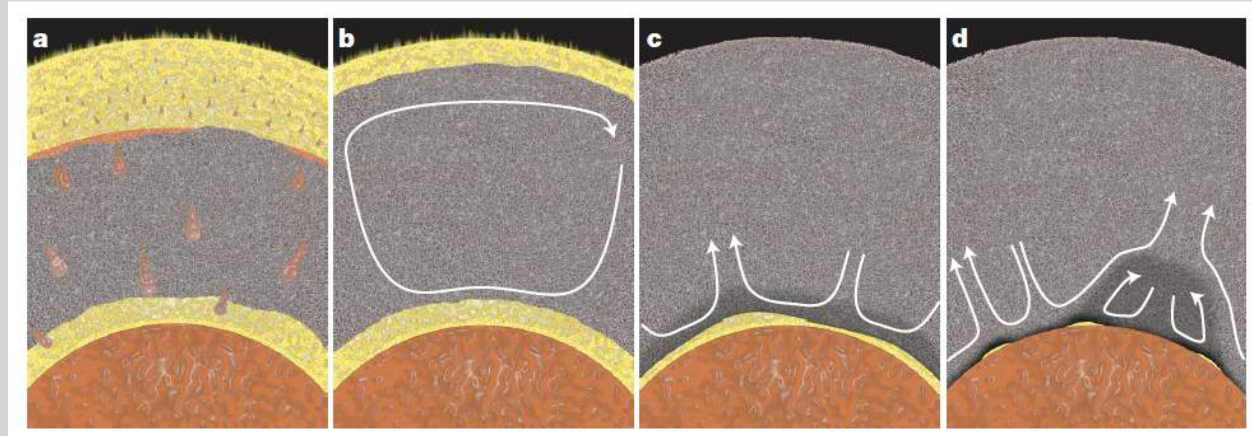
[*Labrosse et al.*, 2015]

Origin of Heterogeneity

Genesis:
- -Primordial
- -Via Convection/Plate Tectonics

Physical Reservoirs of Geochemical Signatures

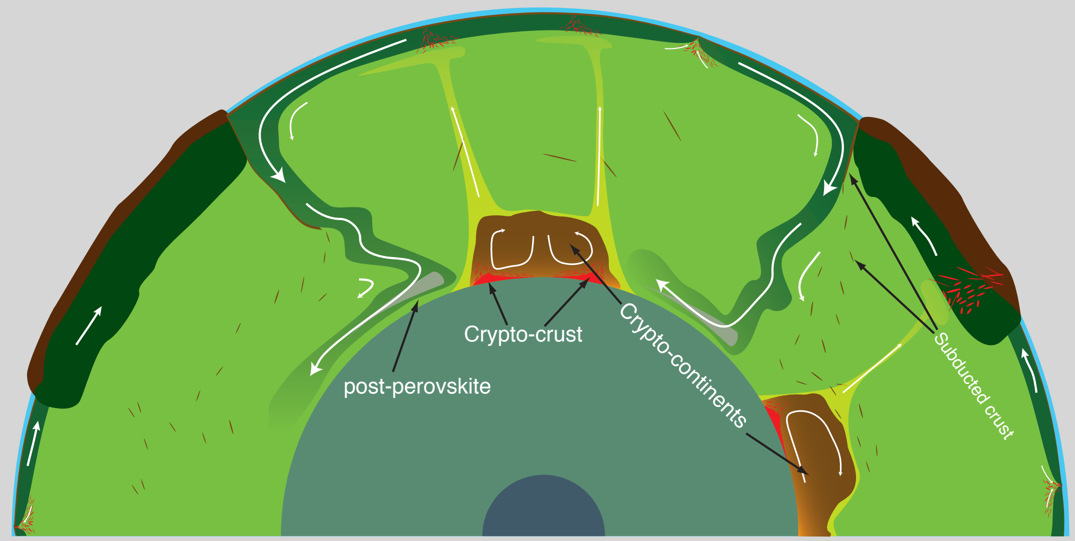
Reservoir for ^{142}Nd?



Labrosse et al., 2007

Signals from primordial magma ocean?

Related to present LLVPs and ULVZs?

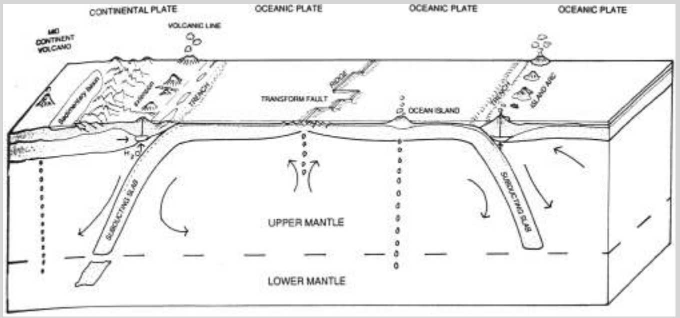


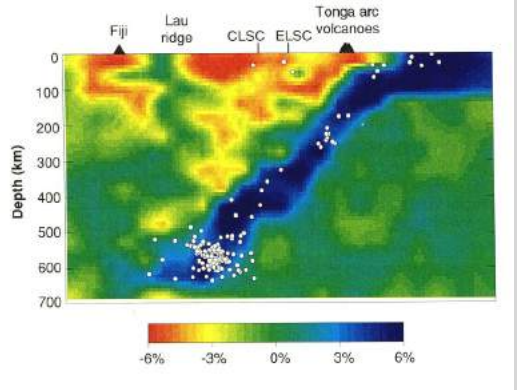
[*Labrosse et al.*, 2015]

Origin of Heterogeneity

Generation (melting) and Destruction (subduction) of Oceanic Lithosphere

Plates ⟷ Mantle Convection





[*Zhao et al.*, 1997]

Continuous generation of dynamical (thermal) + geochemical (compositional) = seismic heterogeneity

[including phase transitions (TZ!!)]

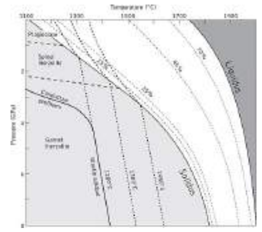
Convection creates and destroys heterogeneity

Melting, Subduction, Stretching

Chemical Heterogeneity ⟷ Seismic

Melting

Decompression Melting



Melting forms oceanic crust (basalt) and depleted residuum (harzburgite)

Densities

basalt ~ 2.9 g/cm^3

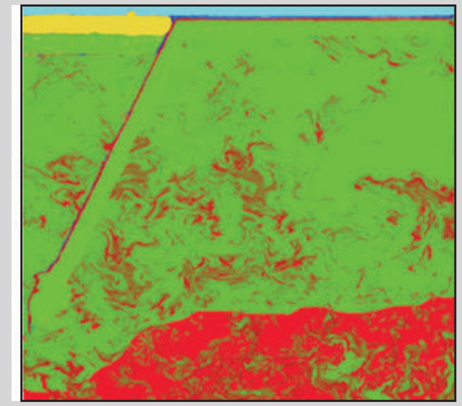
harzburgite ~ 3.2 g/cm^3

lherzolite ~ 3.3 g/cm^3

Oxburgh & Parmentier (1977)

c **Pervasive heterogeneity**

Mechanical mixture

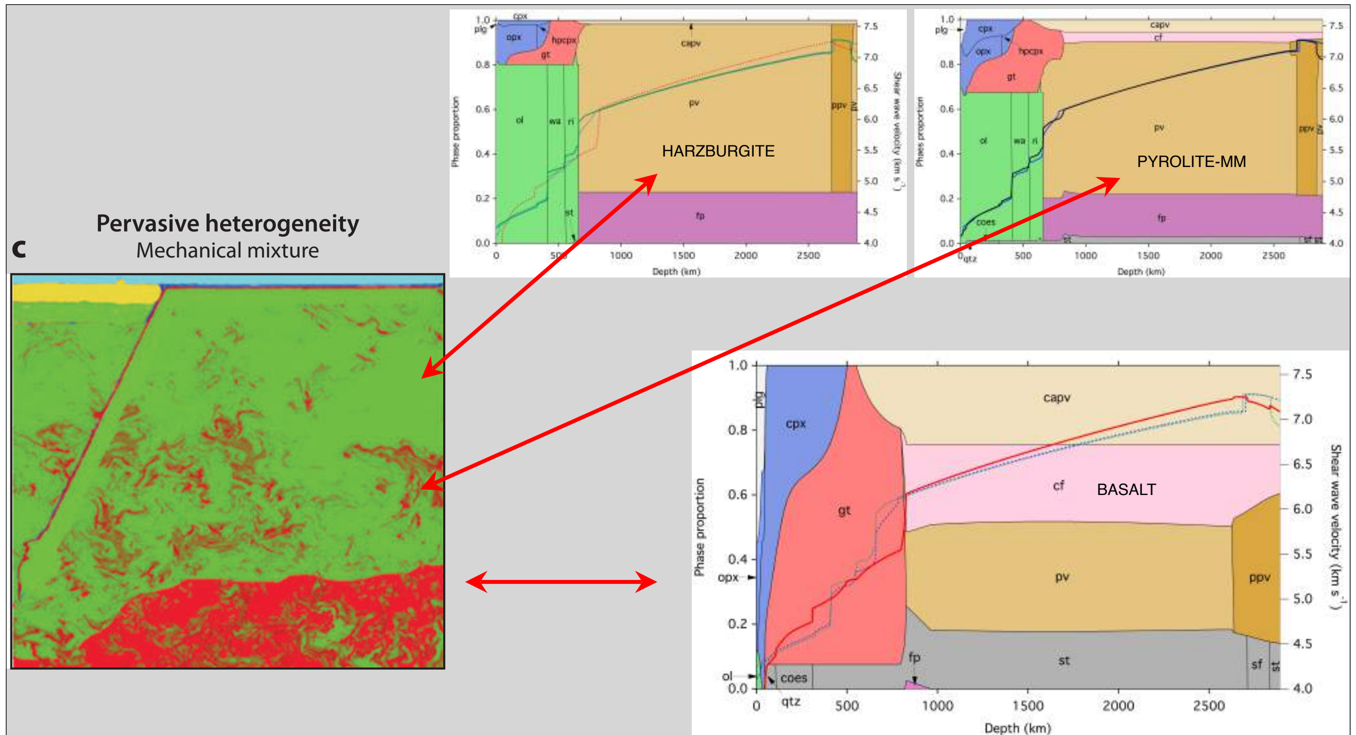


[*Stixrude & Lithgow-Bertelloni*, 2012]

eclogite ~ 3.5 g/cm^3

Mechanical Mixture

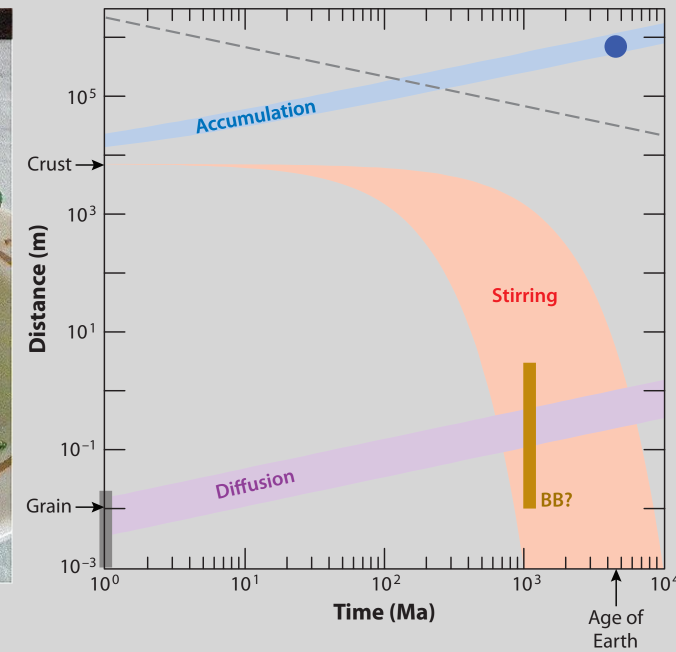
LLVPs - ancient basalt graveyards?
MANTLE-MM of eclogite and harzburgite?



[*Stixrude & Lithgow-Bertelloni*, 2012]

Seismic Signal

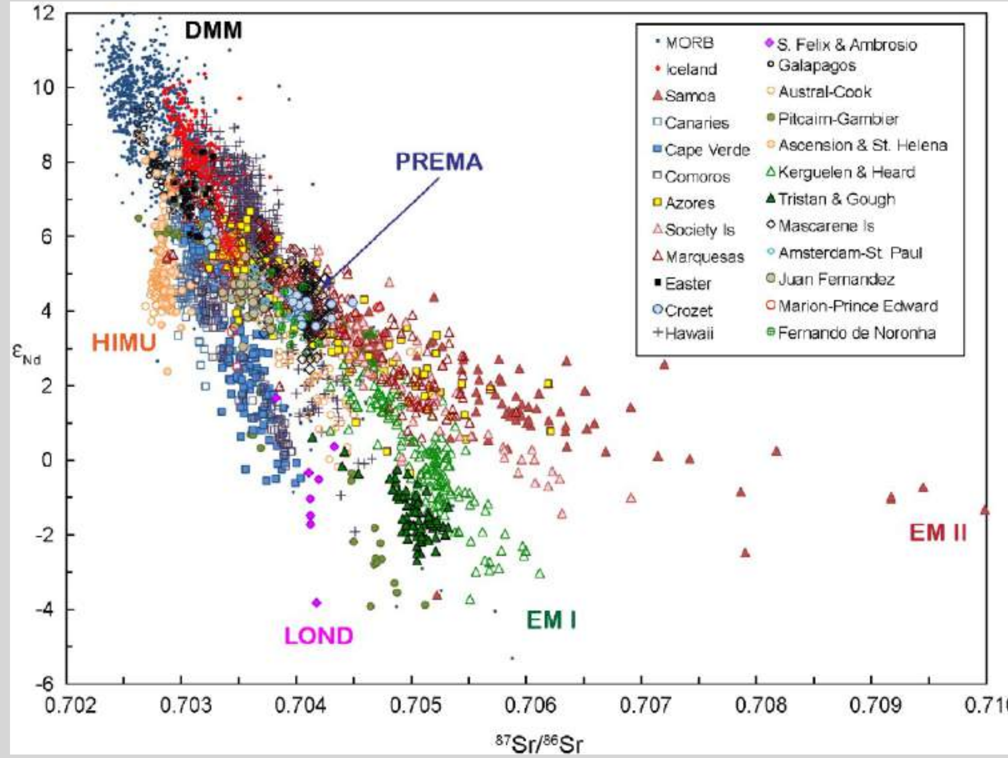
Direct
Scattering



Marble cake mantle

Length scale and survival of heterogeneity in the mantle

Evolution of length scales relevant to the survival of heterogeneity in the mantle. (Red) Flow-induced thinning of heterogeneity with initial thickness equal to that of present day oceanic crust (7 km) assuming exponential thinning (see text) and values of the strain rate ranging from ε˙ = u/L = 6 × 10−16 s−1 to one-tenth this value to account for the possible effects of pure versus shear strain partitioning and more sluggish convection in the lower mantle, where u is present-day average plate speed (5.5 cm year−1) and L is the depth of the mantle (2891 km). (Purple) Length scales over which chemical diffusion is operative with values of the effective diffusion coefficient appropriate to the lower mantle (0.4–7 × 10−18 m2 s−1). The width of the envelope corresponds to a range in oxygen fugacity of six orders of magnitude (Holzapfel et al. 2005). (Blue) The maximum rate of accumulation of a cylindrical pile of basalt with radius = √vhc t, where
v = 1–10 cm year−1 is the sinking velocity, assuming that it separates from harzburgite efficiently at the core-mantle boundary and is not re-entrained in the overlying flow. The dashed gray line shows the radius of a Stokes blob that will traverse half the mantle depth in time t r = 9Lη/4gρt, where η = 5 × 1022 Pa s is the lower mantle viscosity (Lithgow-Bertelloni & Richards 1998), and g is gravitational acceleration for a nominal density contrast ρ = 100 kg m−3. The blue circle represents the thickness of the accumulated pile of basalt in the geodynamic model of Nakagawa et al. (2010). The gold band represents the range of thickness of pyroxenite bands measured in the Beni Bousera (BB) peridotite massif (Pearson & Nowell 2004) and the rhenium-osmium age of melt extraction from the Beni Bousera peridotite (Pearson & Nowell 2004).



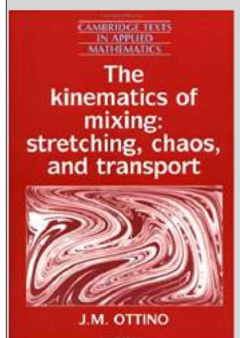
Isotope array

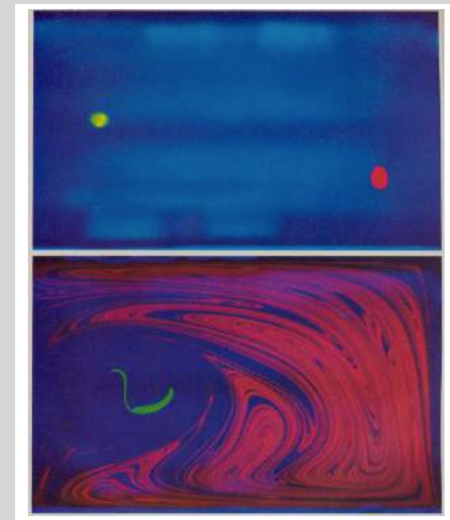
Interpreting requires understanding entrainment and mixing and sampling

“Virtually everyone agrees that mixing is complicated”

J.M. Ottino, Annual Reviews of Fluid Mechanics, 1990

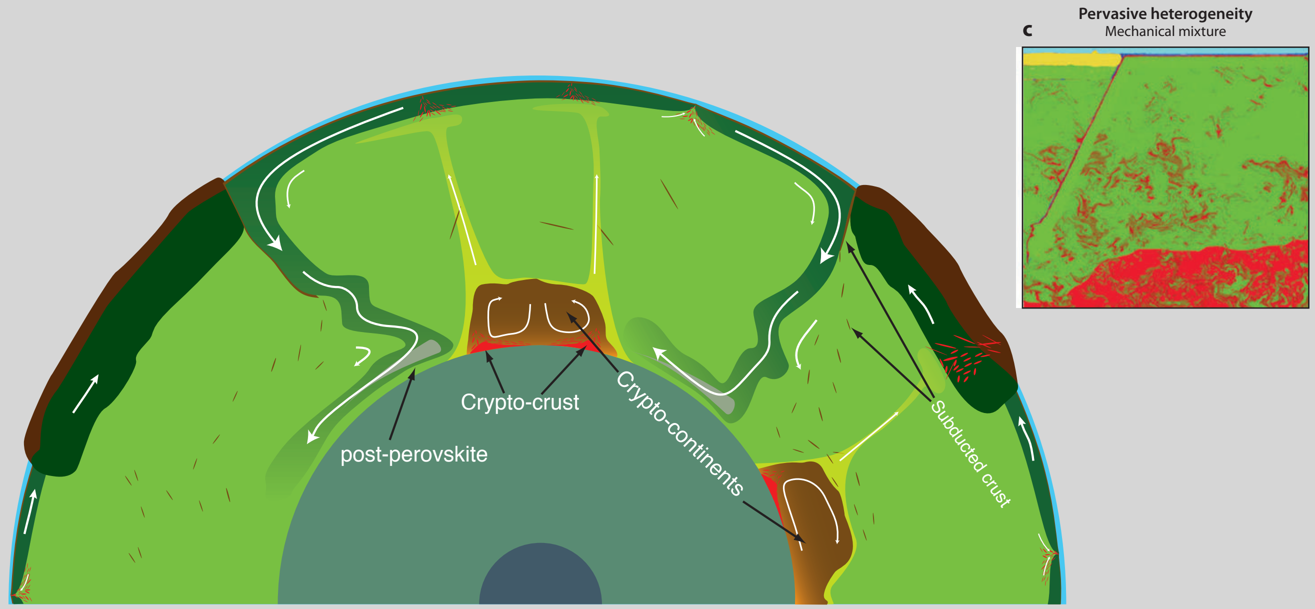
Also watch Michael Manga’s and Louise Kellog’s excellent lectures on Fundamentals of Mixing at CIDER 2012, 2014





Mixing

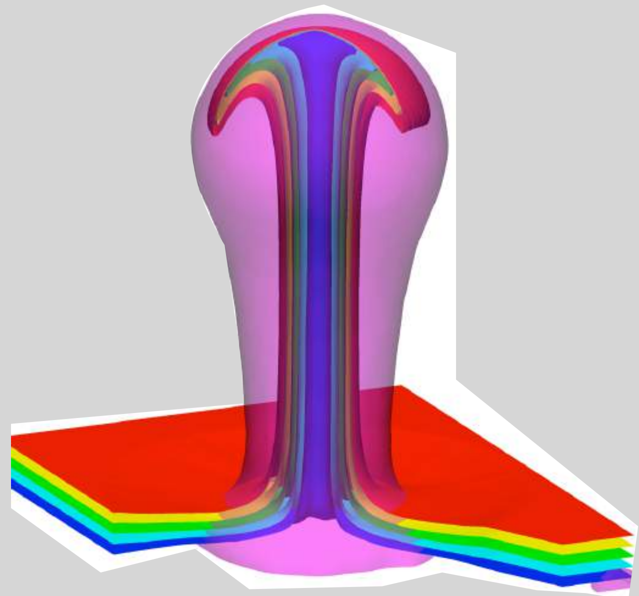
It’s hard….

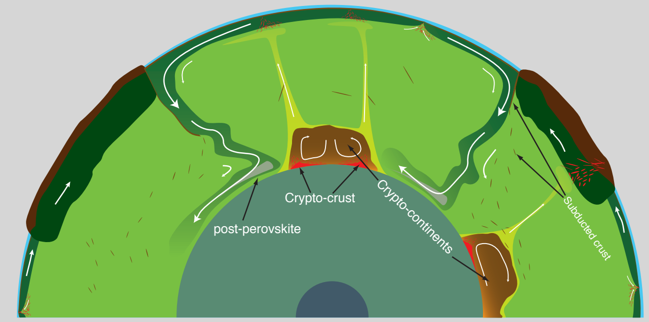


(Labrosse, Hernlund, Hirose, AGU Mon. 2015)

Entrainment, Stirring and Mixing

Entrainment is when a fluid picks up and drags another fluid or a solid





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Entrainment

Definition

Stirring and Mixing: What's the difference?

Stirring is the mechanical motion of the fluid (cause)
stretching and *folding* of material surfaces to reduce length scales

Mixing is the homogenization of a substance
by *stirring* and *diffusion*

Two extremes: Turbulent and laminar mixing

For very viscous flows (mantle) use simple time-dependent flows to create chaotic mixing

Diffusion

The governing equation of the natural diffusion (dispersal) of a substance (heat, dye, chemical)

$$\frac{\partial \theta}{\partial t} = \kappa \nabla^2 \theta$$

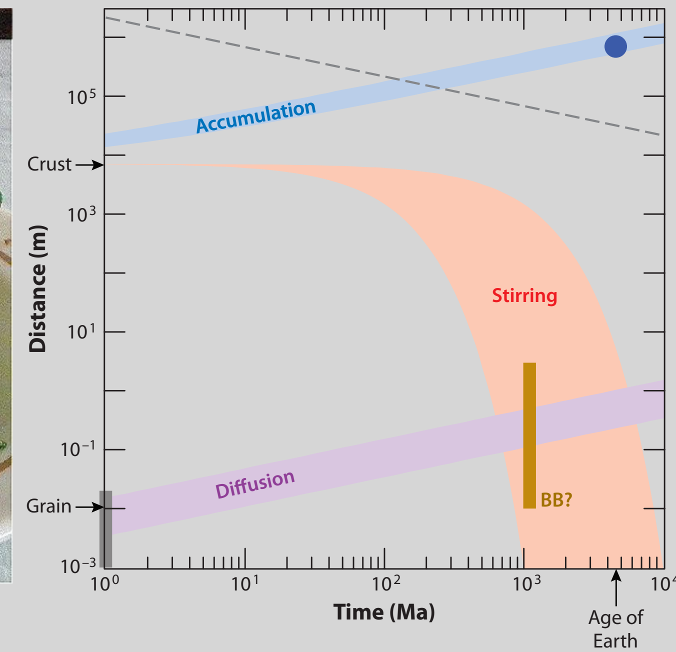
$\theta(\mathbf{x},t)$ concentration of something we need to mix

κ is the diffusivity (thermal, chemical)

But natural or molecular diffusion is really slow… so homogenization hard
thermal diffusivity ~10^{-6} m/s^2
chemical diffusivities ~10^{-18-20} m/s^2 (mantle)
~10^{-11} m/s^2 (magma)

$\ell = \sqrt{\kappa\tau}$

~10-20 cm in a 1 Byr



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Advection and Diffusion

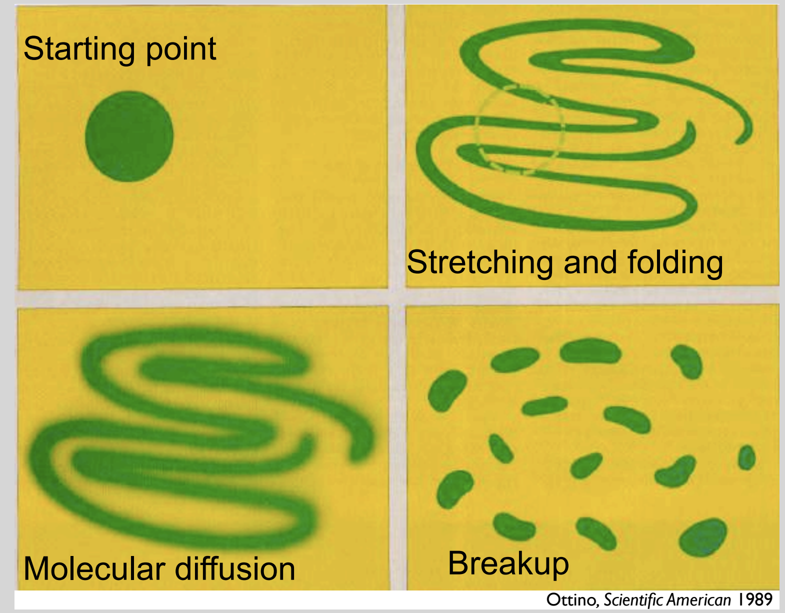
Neglects effect of stirring which creates a flow **v**(**x**,*t*) giving the advection-diffusion equation

$$\frac{\partial \theta}{\partial t} + (\vec{v} \cdot \nabla)\theta = \kappa \nabla^2 \theta$$

Advection term massive effect by increasing spatial gradients of θ

Stirring makes mixing much faster, because it reduces the length scales (stretching, folding)

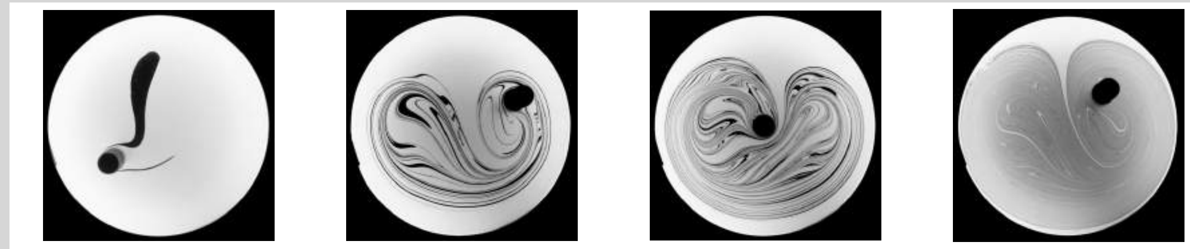
How does mixing happen?



Role of stretching and folding

signature of chaos

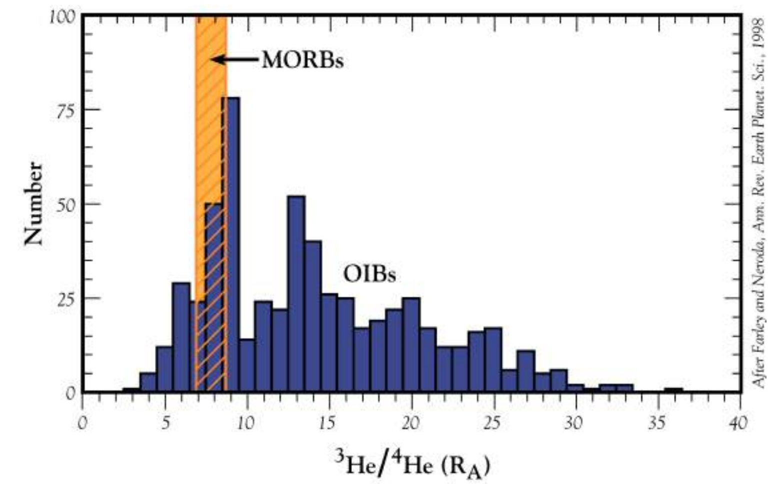
Example: Rod moving in a figure 8 pattern



Stretching and Folding

Some regions remain unmixed

1. Global scale: mantle contains well-mixed regions and heterogeneity



From Michael Manga's 2012 lecture

Mixed vs Unmixed Regions

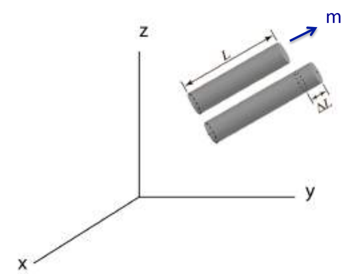
Islands

How to characterize mixing?

Stretching: deformation of material filament from $d\boldsymbol{L(0)}$ to $d\boldsymbol{L(t)}$ given by deformation tensor (related to the velocity)

Strain rate of fluid element L(t)

$$\dot{\Delta} L/L(t) = \mathbf{m}\cdot(\dot{\mathbf{e}}\cdot\mathbf{m})$$



Length Stretching

$$\lambda = \lim_{L(0)\to 0} L(t)/L(0)$$

Rate of Stretching

$$\frac{D\lambda}{Dt} = \frac{\dot{L}(t)}{L(0)} \Rightarrow \frac{1}{\lambda}\frac{D\lambda}{Dt} = \frac{D\ln\lambda}{Dt} = \mathbf{m}\cdot(\dot{\mathbf{e}}\cdot\mathbf{m})$$

Strain-rate tensor $\dot{e} = \frac{1}{2}[\nabla\mathbf{v} + (\nabla\mathbf{v})^T]$

Stretching Tensor

Note: I'll be using x instead of L

How to characterize mixing?

Stretching Efficiency:

$$e_\lambda = \frac{D \ln \lambda / Dt}{(\dot{e} : \dot{e})^{1/2}} \leq 1$$

For simple shear e_λ -> 0 at large times
For pure shear e_λ -> 2/3

What does it mean?

THAT IT DEPENDS ON THE FLOW TYPE!

Lyapunov Exponent: $\sigma_{max} = \lim_{t \to \infty} \frac{1}{t} \ln \frac{|\delta \boldsymbol{x}|}{|\delta \boldsymbol{x}(0)|}$

Not the same as e_λ because the strain rate tensor varies in space and time. There is more than one σ at a given point we only worry about the largest one.

Stretching Efficiency | Depends on Flow

Average rate of stretching experienced by a region of fluid over time span to to t

Lyapunov exponent is a quantity that characterizes the rate of separation of infinitesimally close trajectories. Quantitatively, two trajectories in phase space with initial separation diverge where λ is the Lyapunov exponent.

Lets consider **linear** 2D flows in the x-y plane

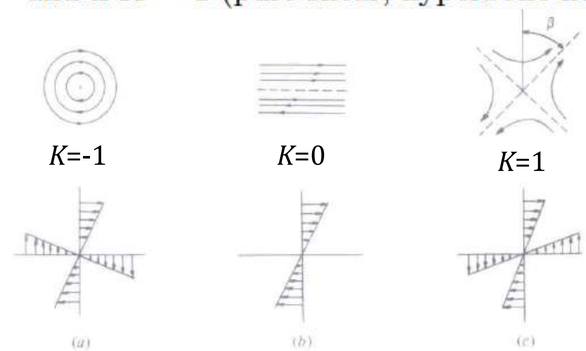
$$v_x = Gy \quad \text{and} \quad v_y = KGx$$

For long times, if $K = 0$ (simple shear)

$$\lambda \sim Gt$$

and if $K = 1$ (pure shear, hyperbolic flow)

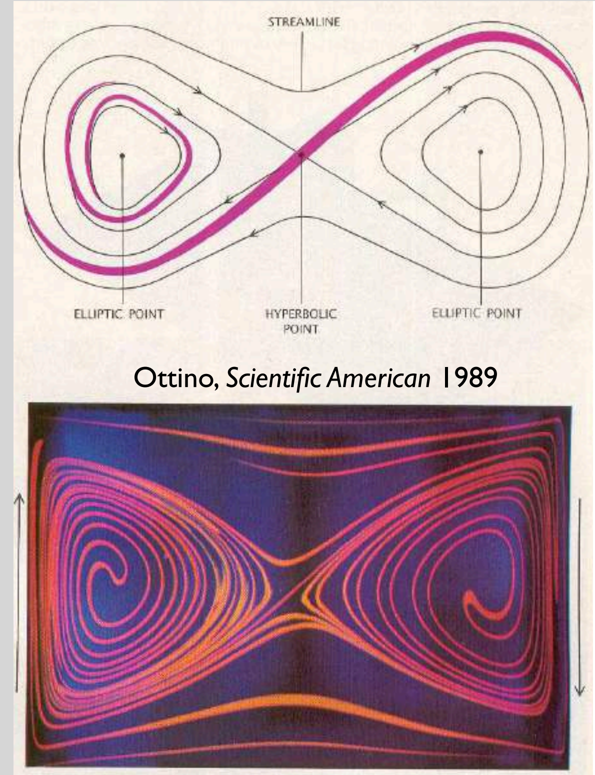
$$\lambda \sim e^{Gt}$$



In a more complex flows, regions with pure shear (hyperbolic streamlines) will cause most of the *stretching*

From Michael Manga's 2012 lecture

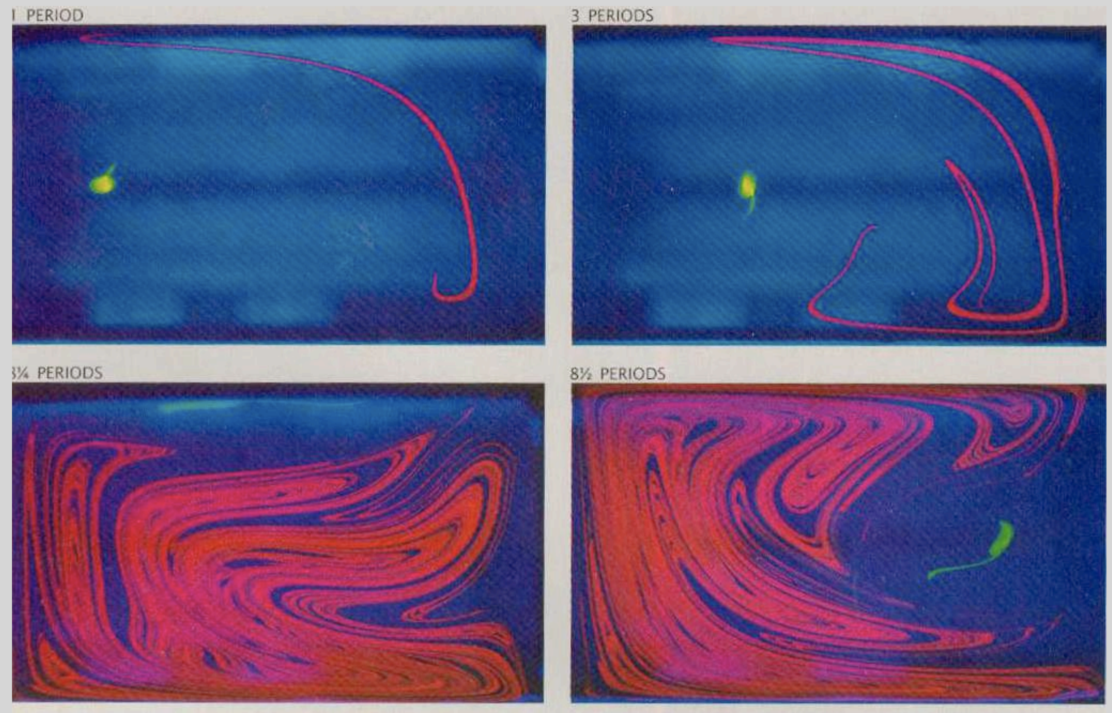
Dependence on Flow Type



Ottino, *Scientific American* 1989

Elliptic and Hyperbolic points

Steady 2D flows don't mix well…
but add time-dependence



Time-dependence

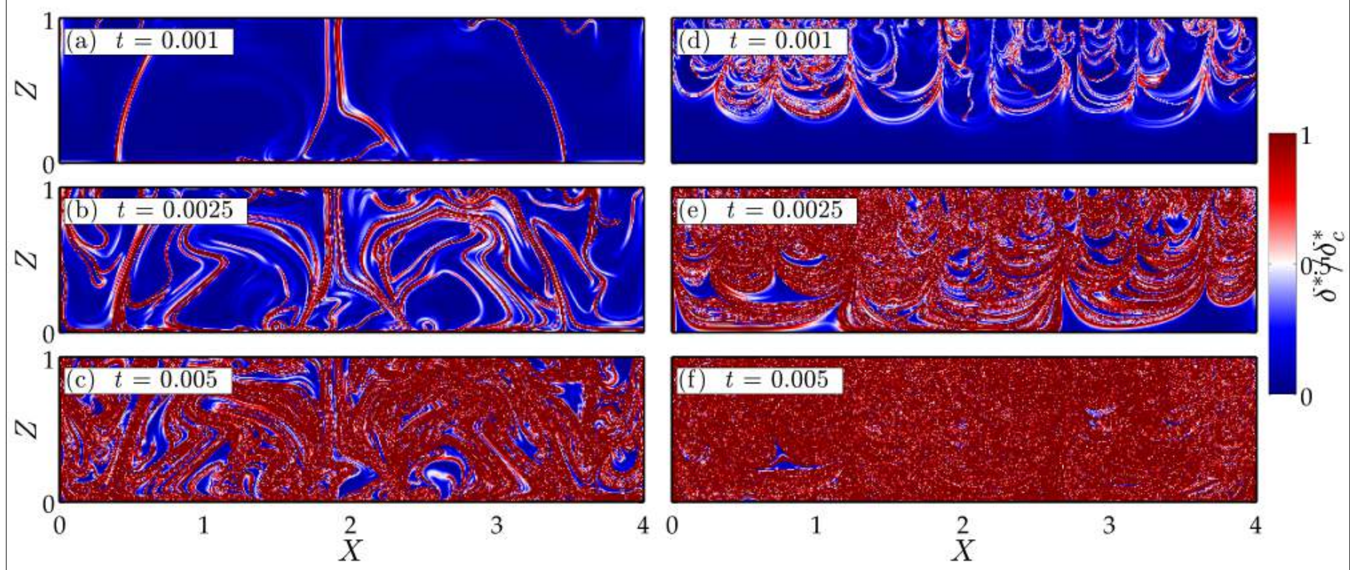
Well mixed and not well mixed regions coexist

Stirring can produce complex structures and
mixed and *unmixed* islands

Chaotic Flow and Mixing
by *stretching* and *folding*
tracers *sensitive to initial conditions*
presence of special points
produces horseshoe maps

Dependence on type of heterogeneity
active (chemical, rheological)

Effects of stirring



Global vs Local Mixing

Effect of viscous increase

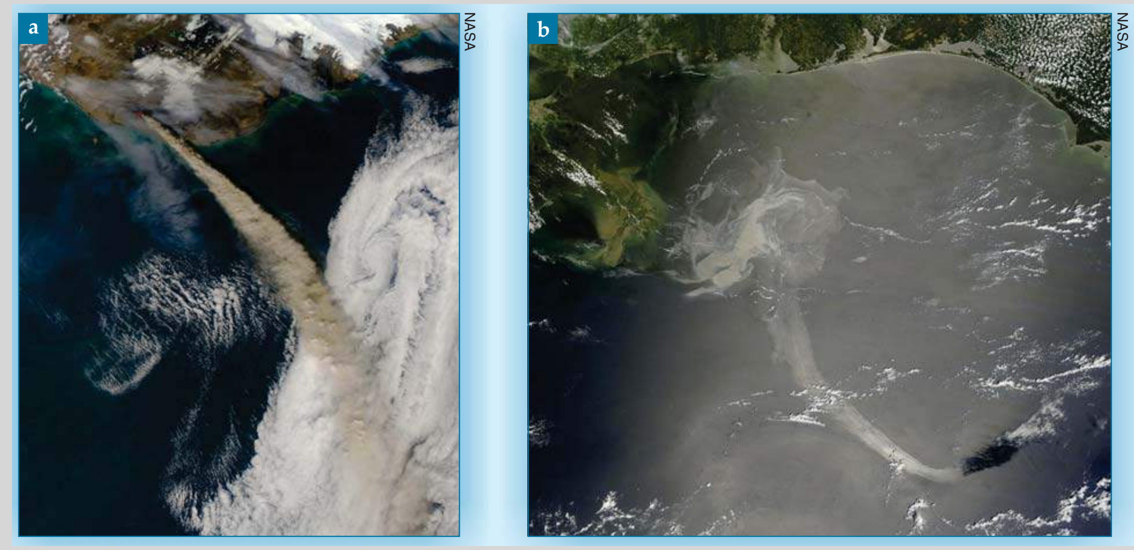
Characterization of Structure

"Important to distinguish between mixing measure and the process producing mixing… The measure should be selected according to the application, and the measurements should be related to the fluid mechanics."
Ottino, Kinematics of Mixing, 1989

e and σ characterize effectiveness of a given *flow* at stirring

Other measures can be used to characterize observed structures (fractal analysis, spectral)

Measures of Mixing



[*Peacock and Haller*, 2013]

http://shaddenlab.berkeley.edu/uploads/LCS-tutorial/overview.html

Lagrangian Coherent Structures

Key material lines that organize fluid flow

Generally speaking, the LCS approach provides a means of identifying key material lines that organize fluid-flow transport. Such material lines account for the linear shape of the ash cloud in figure 1a, the structure of the oil spill in 1b, and the tendrils in the spread of radioactive contamination in 1c. More specifically, the LCS approach is based on the identification of material lines that play the dominant role in attracting and repelling neighboring fluid elements over a selected period of time.

- Basic premise
  - Non-linear equations hard
  - Ignore struggle for particular analytical solution
  - Focus on behavior of all solutions
- Stable and unstable manifolds organize state space

Dynamical System

$$\begin{aligned} \dot{x} &= x + y \\ \dot{y} &= 4x - 2y \end{aligned}$$

$$\dot{\boldsymbol{x}} = \boldsymbol{J}\boldsymbol{x}$$

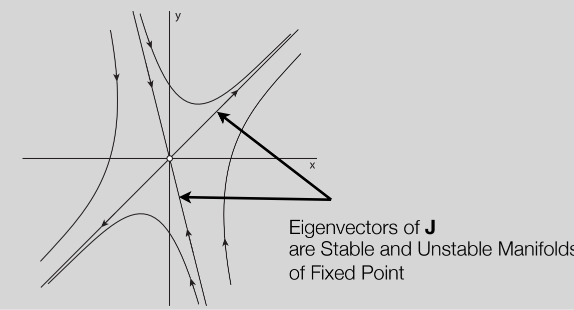
Fixed Point

$$\boldsymbol{x} = (0,0) \Rightarrow \dot{\boldsymbol{x}} = (0,0)\ \forall t$$

General Solution

$$\boldsymbol{x}(t) = c_1 \begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{2t} + c_2 \begin{pmatrix} 1 \\ -4 \end{pmatrix} e^{-3t}$$

Phase Portrait



Dynamical Systems

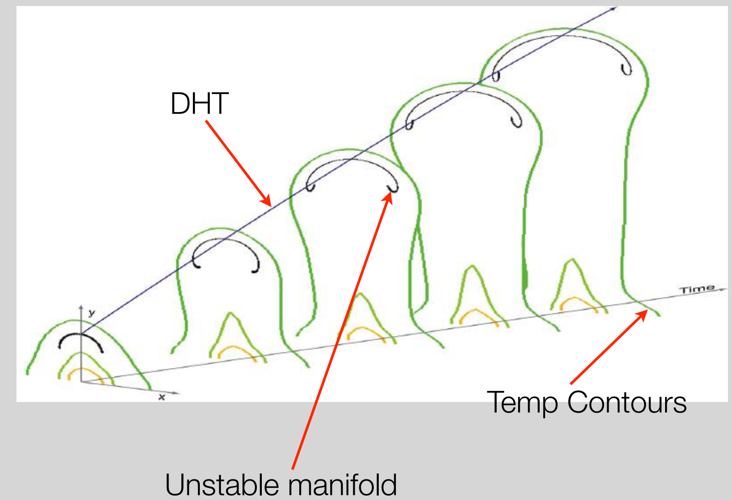
Separatrices
Attracting and Repelling points

A geometric-computational tool has been developed to locate Lagrangian coherent structures, or LCS. This is the concept that generalizes the notion of invariant manifold in dynamical systems to the time dependent case. As with separatrices, LCS are dividing lines between particles with different dynamical fates. An LCS (Lagrangian Coherent Structure) is a ridge in the FTLE field. LCS are time dependent curves in 2d flows and surfaces in 3d flows

- Aperiodic systems have explicit time dependence
- Resulting dynamical system can be made autonomous by adding state variable for time
    - Fixed points vanish
    - Left with distinguished hyperbolic trajectories
        - Distinguished:
            - Behaves like moving fixed point (i.e., a parcel on this trajectory can't get off)
            - Has invariant manifolds (aka, LCS)
            - Other trajectories exponentially approach or recede
        - Hyperbolic: non-zero Lyapunov exponents

$$|\delta \boldsymbol{x}| = |\delta \boldsymbol{x}(0)|\, e^{\sigma t} \qquad \sigma_{max} = \lim_{t \to \infty} \frac{1}{t} \ln \frac{|\delta \boldsymbol{x}|}{|\delta \boldsymbol{x}(0)|}$$

- Aperiodic systems theory is still under much development



FTLE and LCS

large literature

Finite Time Lyapunov Exponent

The average rate of stretching experienced by a region of fluid over the time-span t_0 to t is typically expressed using the Finite-Time Lyapunov Exponent (FTLE), σ_f (Shadden *et al.* 2005). This is found by first finding the flow map:

$$\phi\left(\mathbf{x}, t, t_0\right) = \mathbf{x}\left(\mathbf{x_0}, t, t_0\right), \tag{3.4}$$

which is the position of all tracers at time t which had the initial position, $\mathbf{x}_0$ at time t_0 (with $t_0 < t$). This is in turn used to find the Cauchy-Green deformation tensor

$$C = \left(\nabla\phi\right)^{\top}\left(\nabla\phi\right). \tag{3.5}$$

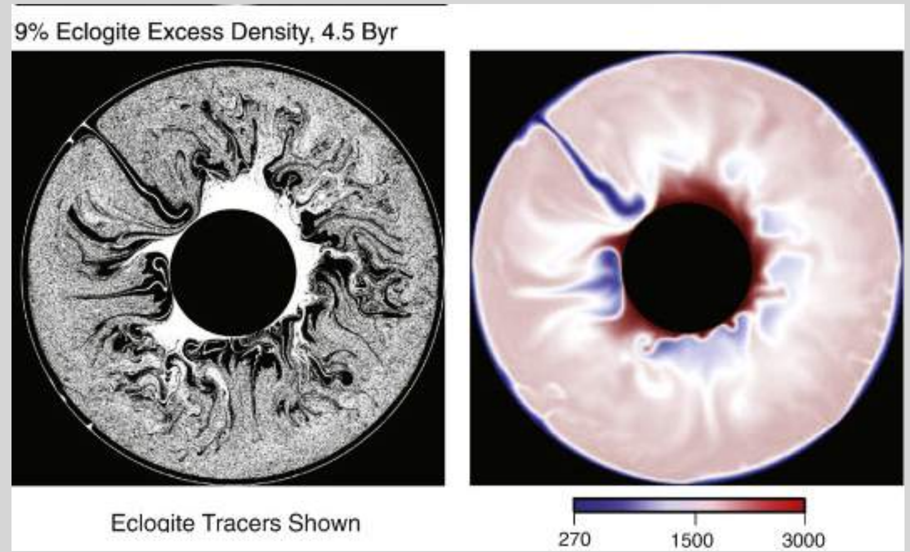
The largest real eigenvector of C, λ_{max} represents the maximum strain. Using this information, the FTLE can be calculated as

$$\sigma_f\left(\mathbf{x}, t, t_0\right) = \frac{1}{2(t - t_0)} \log \lambda_{max}. \tag{3.6}$$

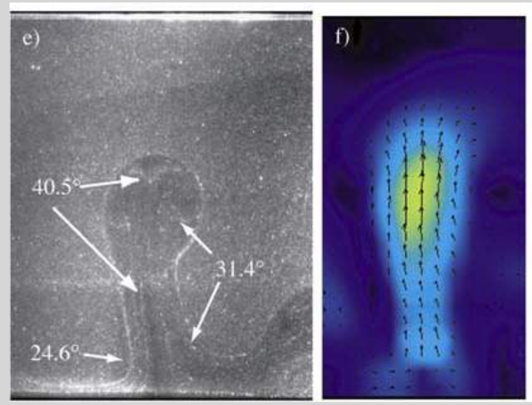
$$\delta^* = \frac{\delta(t)}{\delta(t_0)} = e^{\sigma_f (t - t_0)},$$

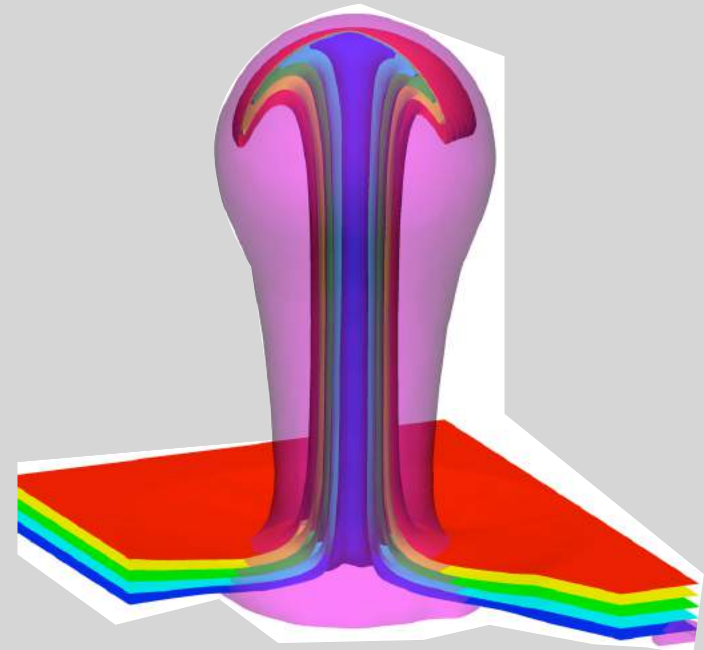
In chaotic systems (as occurs in the mantle), a local region of heterogeneity will be stretched as where delta is the length of the filament of fluid
Thus $_f$ represents the average rate of stretching experienced by a region of fluid which originated at position x over the time-span t_0 to t.

FTLE | How to compute



Advecting Tracers



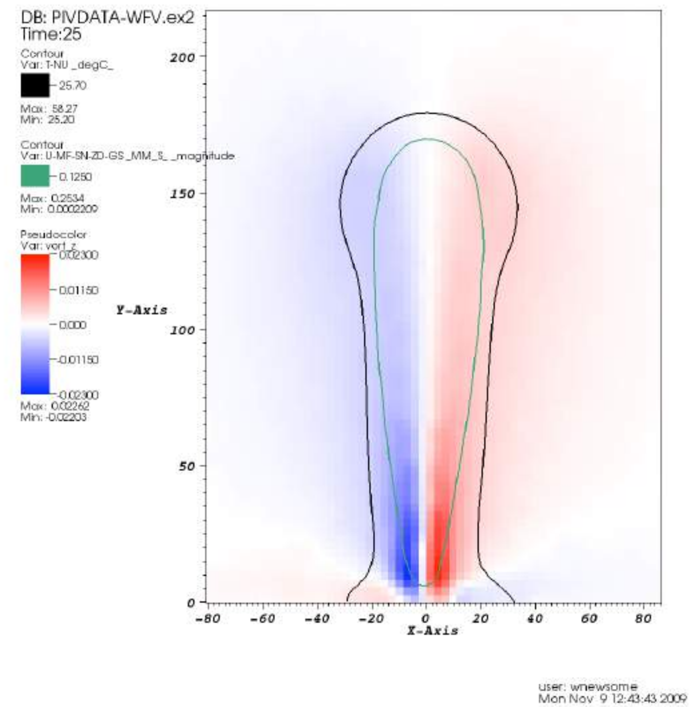


Thermal plumes

Geophysical background

What is a plume?

- To formalize dynamical interaction of plume with surroundings, we need
  - Definition of plume
  - Definition of surrounding
- Our approach
  - Define plume head using dynamical systems concepts
  - Lagrangian Coherent Structures (LCS)
    - Stable and Unstable



Degree to which LCS approximate invariant manifolds is still under development. Is known that regions of high shear will produce high FTLE fields.

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  - D
  - D
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  - La St
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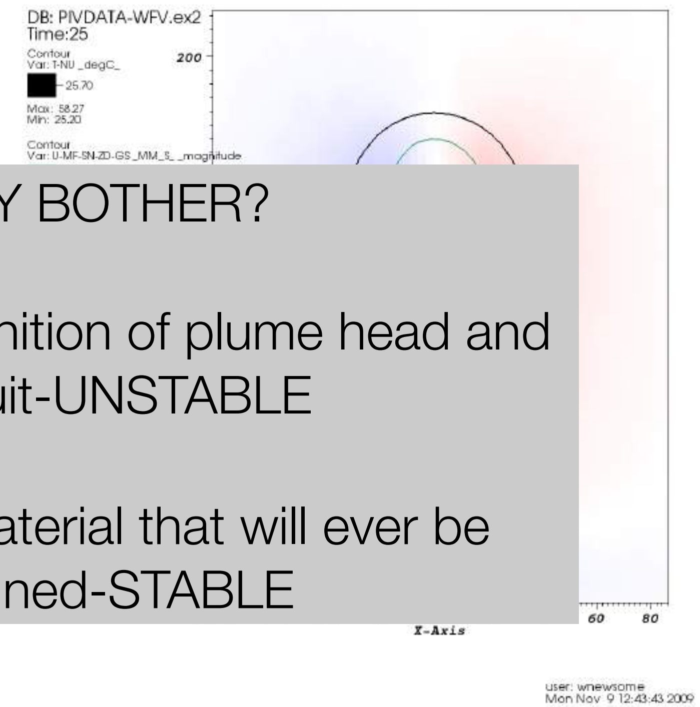


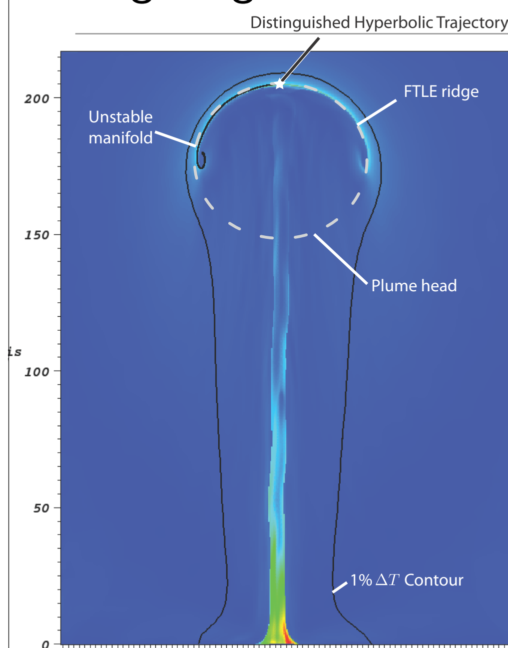
WHY BOTHER?

OBJECTIVE definition of plume head and conduit-UNSTABLE

Define ALL material that will ever be entrained-STABLE

Degree to which LCS approximate invariant manifolds is still under development. Is known that regions of high shear will produce high FTLE fields.

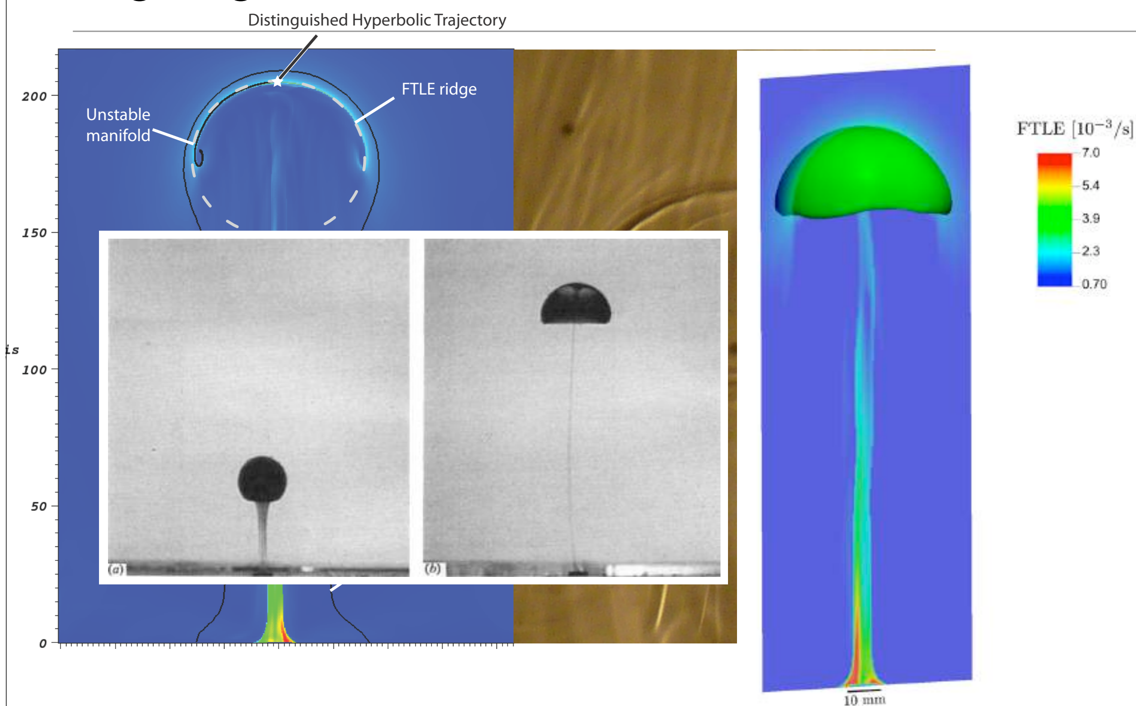
Lagrangian Coherent Structures and Manifolds



Dynamical systems theory provides a robust definition of plume head and source material. The ***unstable*** invariant manifold of the distinguished hyperbolic trajectory at leading edge of the upwelling. The ***stable*** manifold defines all material that will ever be entrained (source)

- Separates flow field into regions with distinct dynamics
- Attract and stretch along manifold (unstable) or repel (stable) nearby fluid elements.

Lagrangian Coherent Structures and Manifolds



des a robust definition
rial. The ***unstable***
juished hyperbolic
upwelling. The ***stable***
it will ever be
entrained (source)

- Separates flow field into regions with distinct dynamics
- Attract and stretch along manifold (unstable) or repel (stable) nearby fluid elements.

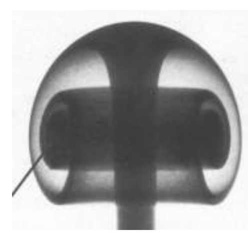
Injection plume vs localized heat source

$$Ra = \frac{\alpha g Q d^2}{\kappa^2 \mu c_p}$$

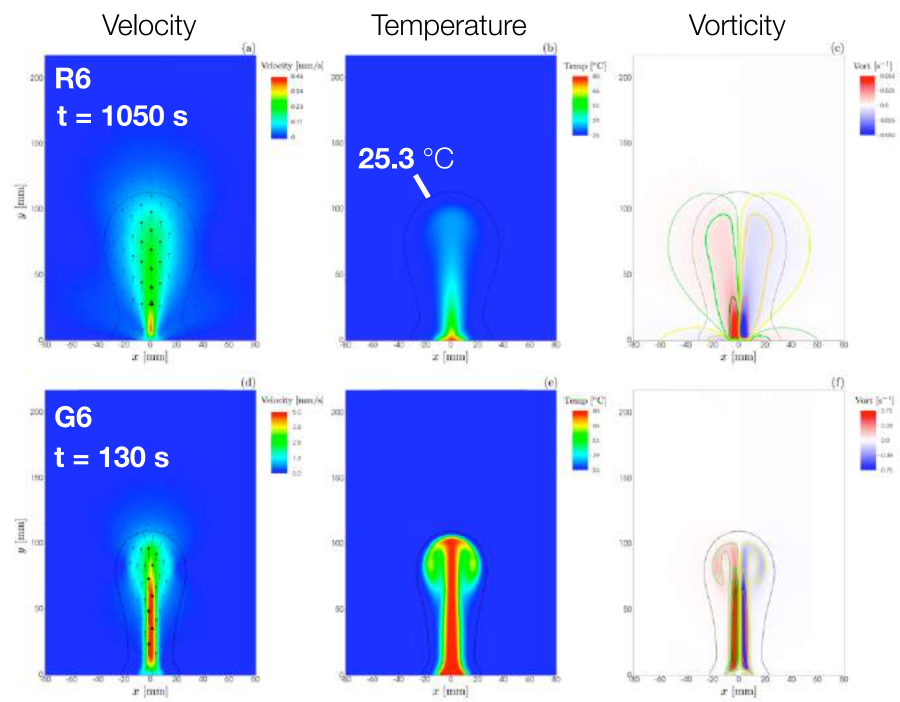
$$Ra(\mathrm{R6}) = 5 \times 10^5$$

$$Ra(\mathrm{G6}) = 2 \times 10^7$$

- Comparison of numerical models
- Both use 80 °C syrup
- Same initial conditions
- Same boundary conditions except
  - G6 upper surface permits outflow on perimeter
  - G6 upper surface temperature floats
- G6
  - Injection rate: 0.3 cm³/s
  - Nozzle: ⌀ 20 mm



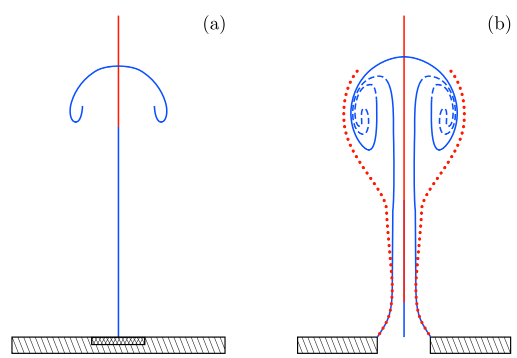
Griffiths & Campbell 1990

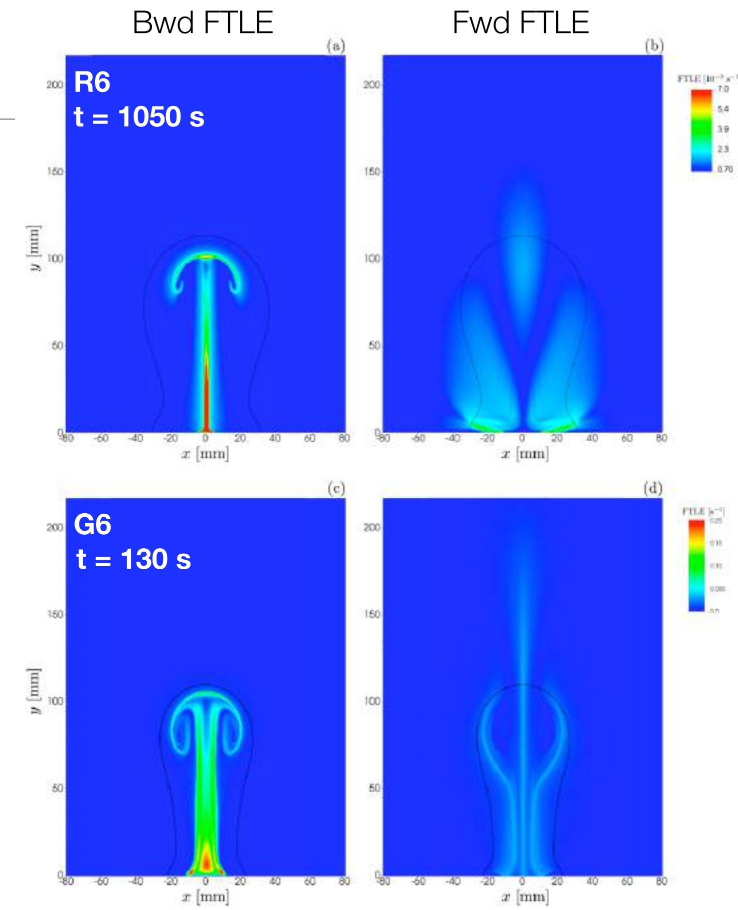


G&C injection rate, Peter's nozzle size (G&C used ⌀ 0.6 cm)
Very distinct differences: v_l 10x, head vorticity 20x greater, head is hotter (my head 33 degC)
Centerline velocity is not monotonic above 30 mm for G6

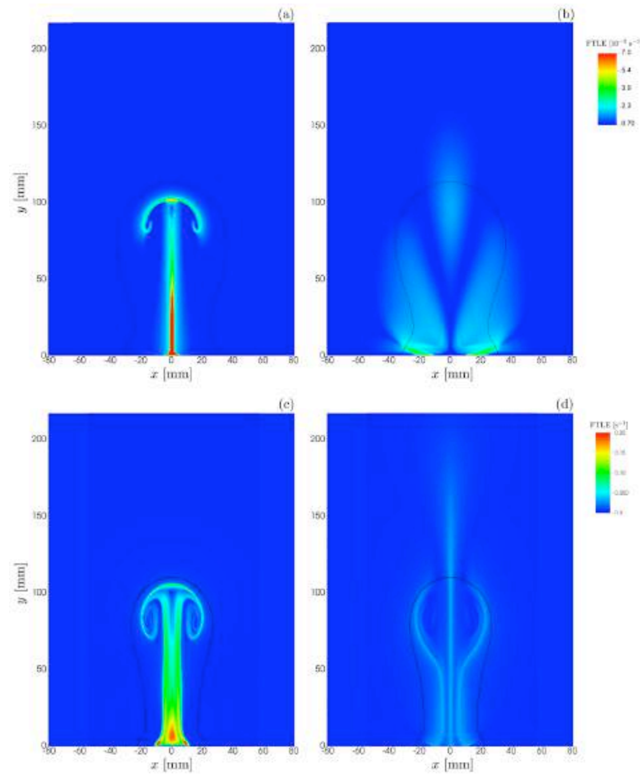
The LCS

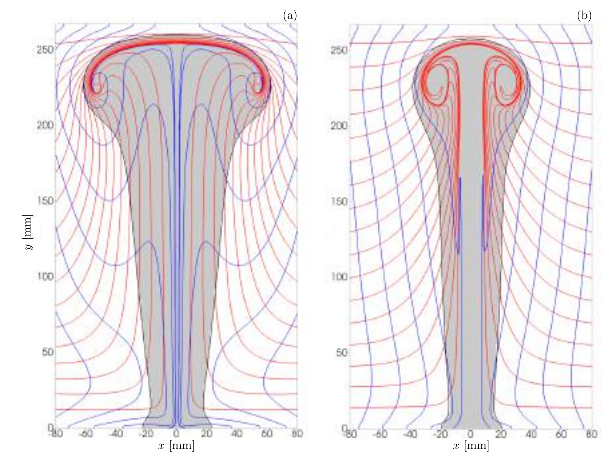
- Two cases are very different
- G6 has
  - Bwd-time LCS surrounding injected mass
  - Fwd-time LCS shielding head





Injection vs Thermal





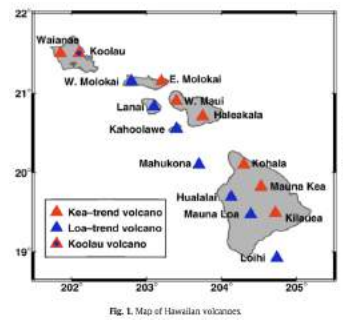
- Mantle plumes operating similarly to the injection plume have acquisition flexibility
- Mantle plumes operating similarly to experimental cases are images of the source

Mantle plumes akin to our cases N1-N6
Head composition dominated by mass from lowermost 600 km
Head inefficient at incorporating overlying material
Overlying heterogeneities confined to outer perimeter of head
If mechanical mixture of eclogite and peridotite required for partial melting, must be characteristic of source
Mantle plume akin to injection plume
Head very efficient at incorporating overlying material
Can acquire signature needed during ascent
Material well-stirred
40% of total head mass derived from depth ≤ 1300 km.

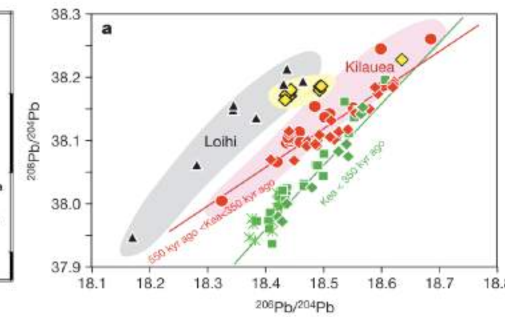
How does the flow transform the unit sphere

- Motivation: Can we use the spatial arrangement and shape of surface observations to constrain
  - transport mechanism
  - mass origin
- Small scale variation in Pb isotope data
  - 350 - 550 kyr Mauna Kea lavas are isotopically similar to present day Kilauea
  - Pancakes or filaments

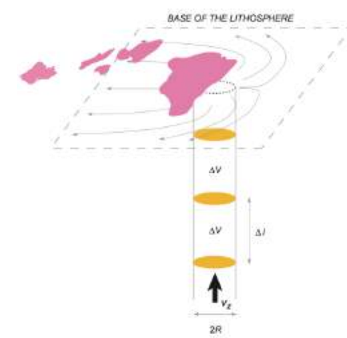
Farnetani & Hofmann 2010



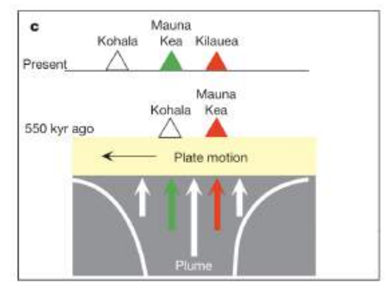
Abouchami *et al.* 2005



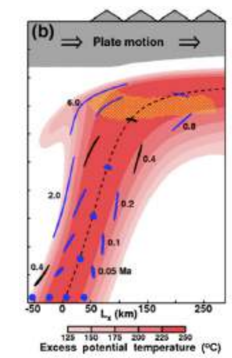
Blichert-Toft *et al.* 2003



Abouchami *et al.* 2005



Farnetani & Hofmann 2010



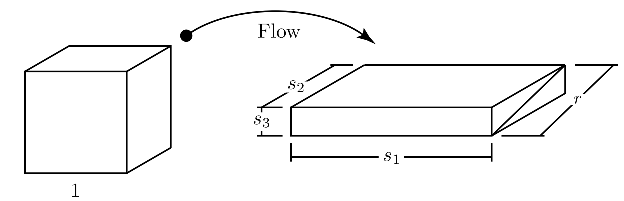
3 Ma Hi started producing lavas with two distinct isotopic trends (Kea and Loa)
HSDP data indicates that small scale variation also exists
Launching spheres is tedious and we may miss a lot
Can we construct a predictive map of how the flow transforms all fluid elements

Transforming the unit sphere

- Dimensionality of LCS provides some insight, but
  - Not all fluid elements interact with LCS
  - Not all interacting fluid elements are transformed the same
- Shape metric Ψ classifies dimensionality of deformed sphere
  - 1D line
  - 2D sheet
  - 3D sphere
- Take s_i as principal stretches

$$\zeta(t) = \frac{\|\delta \boldsymbol{x}(t)\|}{\|\delta \boldsymbol{x}_0\|} = \frac{\sqrt{\delta \boldsymbol{x}_0^T \left(\boldsymbol{\nabla}_0 \boldsymbol{F}\right)^T \boldsymbol{\nabla}_0 \boldsymbol{F} \delta \boldsymbol{x}_0}}{\|\delta \boldsymbol{x}_0\|} = \frac{\sqrt{\delta \boldsymbol{x}_0^T \boldsymbol{M} \delta \boldsymbol{x}_0}}{\|\delta \boldsymbol{x}_0\|}$$

$$\boldsymbol{M} = \boldsymbol{M}(t) \equiv \left(\boldsymbol{\nabla}_0 \boldsymbol{F}\right)^T \boldsymbol{\nabla}_0 \boldsymbol{F}$$



$$\Psi = \frac{r^2}{s_1^2} \quad r = \sqrt{s_2^2 + s_3^2} \quad s_1 \geq s_2 \geq s_3$$

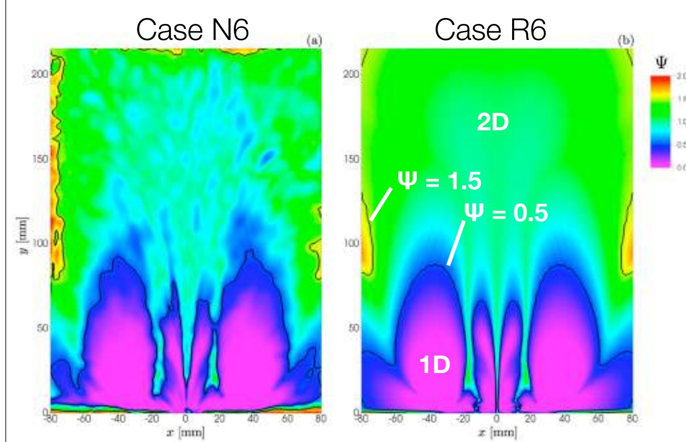
$$0 \leq \Psi \leq 2$$

Shape	Ψ
Sphere (3D)	2
Sheet (2D)	1
Pencil (1D)	0

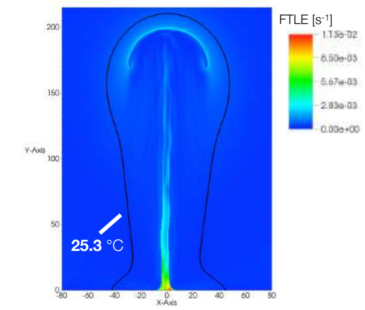
Shape metric for plumes N6 and R6

- Computed using integration time τ = 2000 s
- Predicts how 2000 s of flow will transform infinitesimal spherical mass

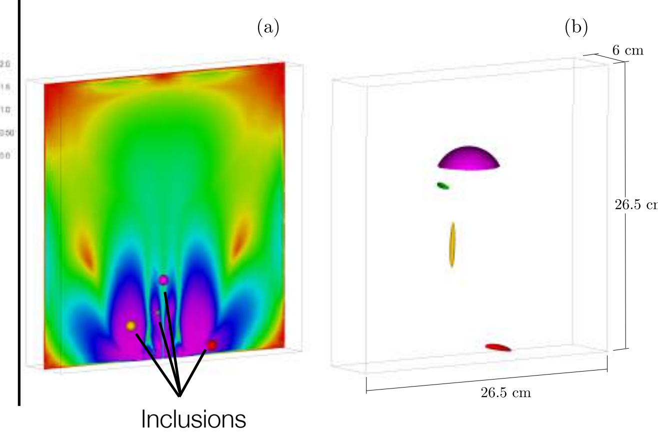
t = 0 s



Plume state at t = 2000 s

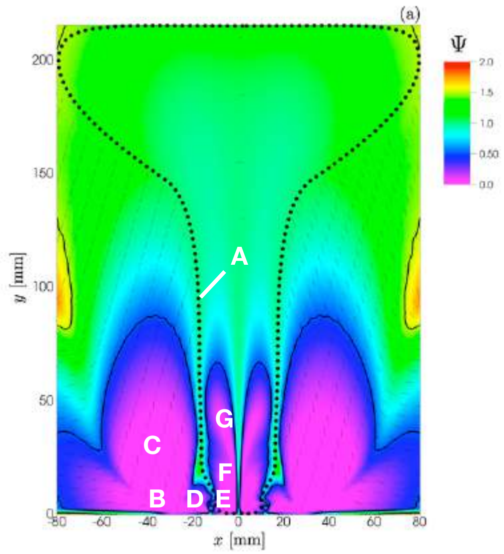


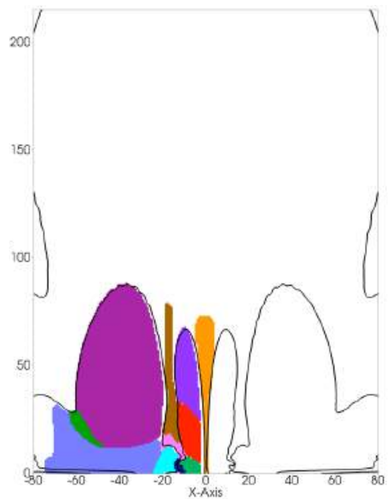
Transformation of 4 macroscopic inclusions

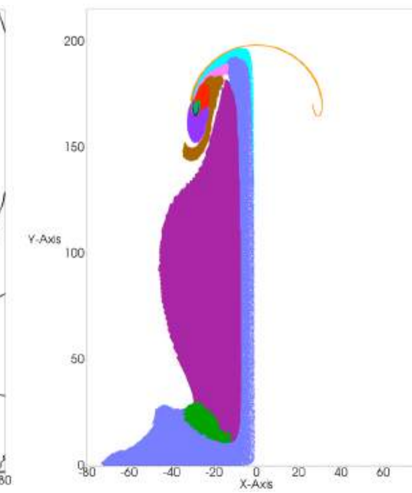


Notice the pockets, there seems to be structure to the field.

Evolution of material pockets extracted from metric







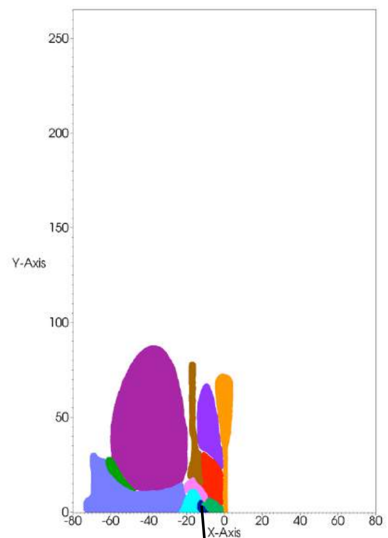
A. Separates mass brought in from above vs below
B. Conduit core
C. Outer conduit
D. Plastered on bottom of LE LCS
E. Head entrain phase 1: Scroll core
F. Head entrain phase 2
G. Head entrain phase 3

Metric

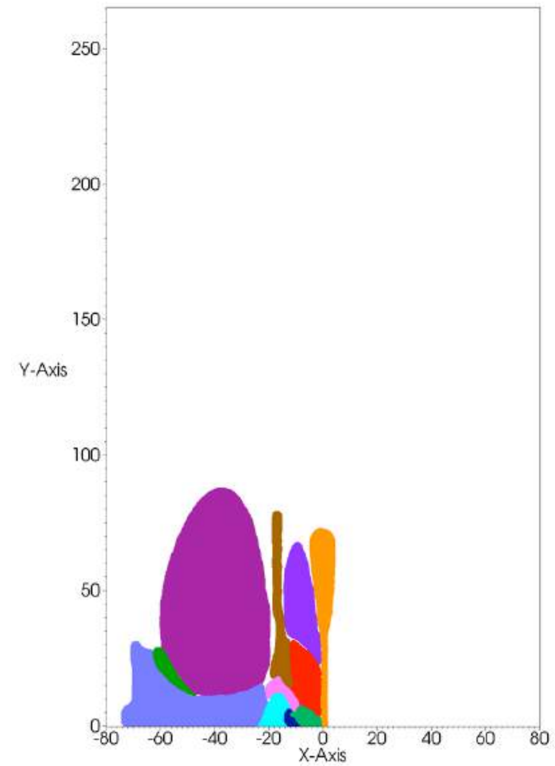
- Elucidates hidden structure
- Permits segregation of head mass entrained from above vs. below

Dotted line encloses max principal stretch perpendicular to view
Lower section segregates mass brought in above vs below

Evolution of material pockets extracted from metric



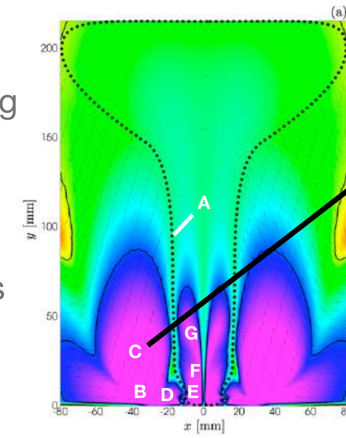
Outer perimeter of rotation

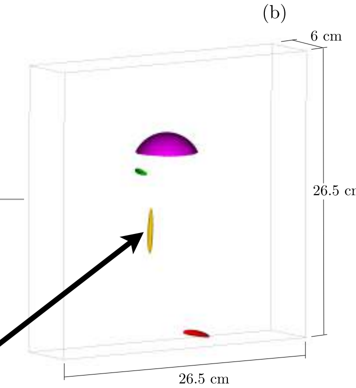


Green rotates

Reflection: plume spatial/temporal variation

- Production of 2D structures limited to mass above the rising plume
- Conduit and head are 1D dominant
- Producing horizontal pancakes in the conduit is difficult





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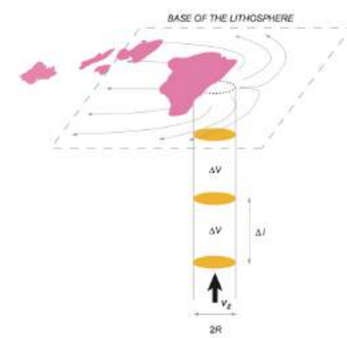
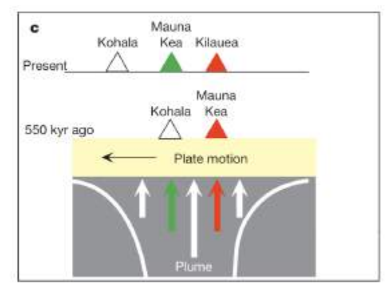
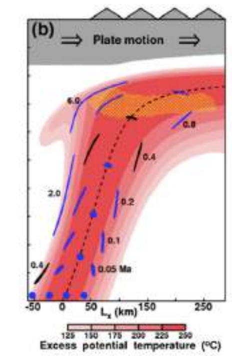
Blichert-Toft *et al.* 2003

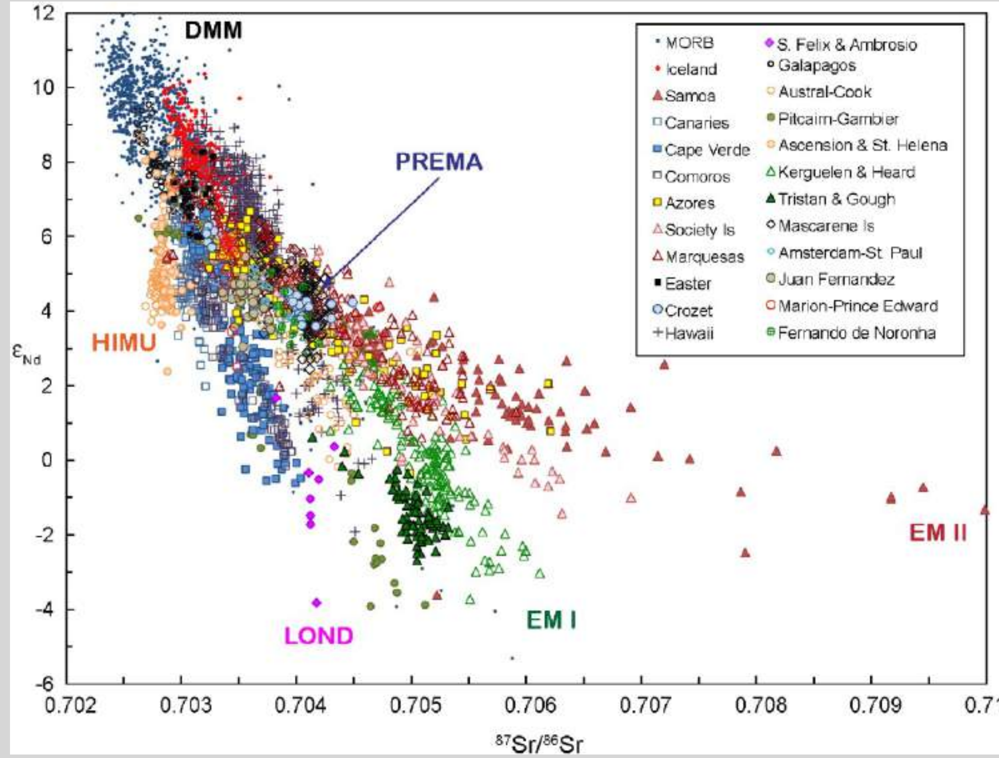


Abouchami *et al.* 2005



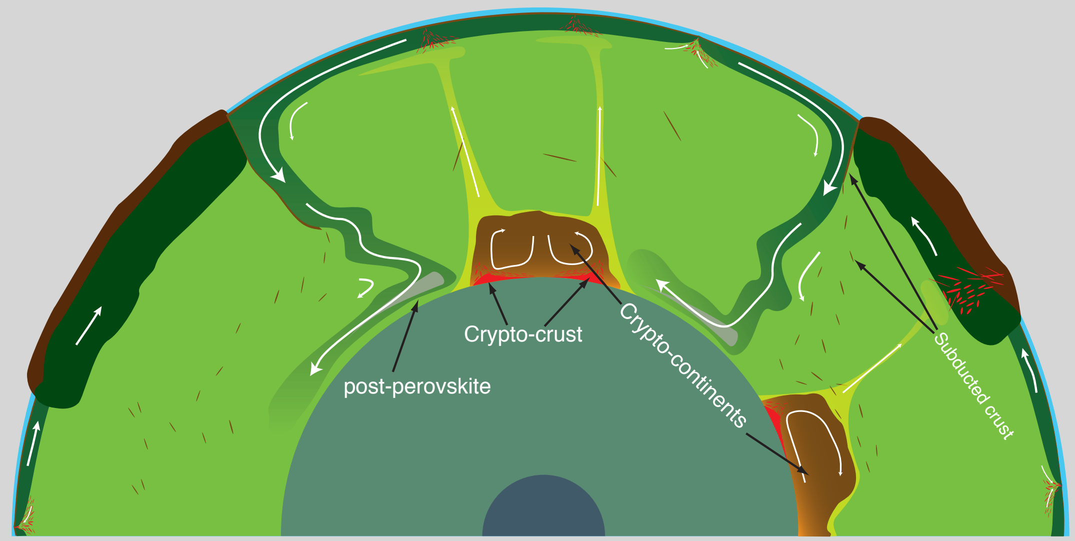
Farnetani & Hofmann 2010





Extricate Meaning

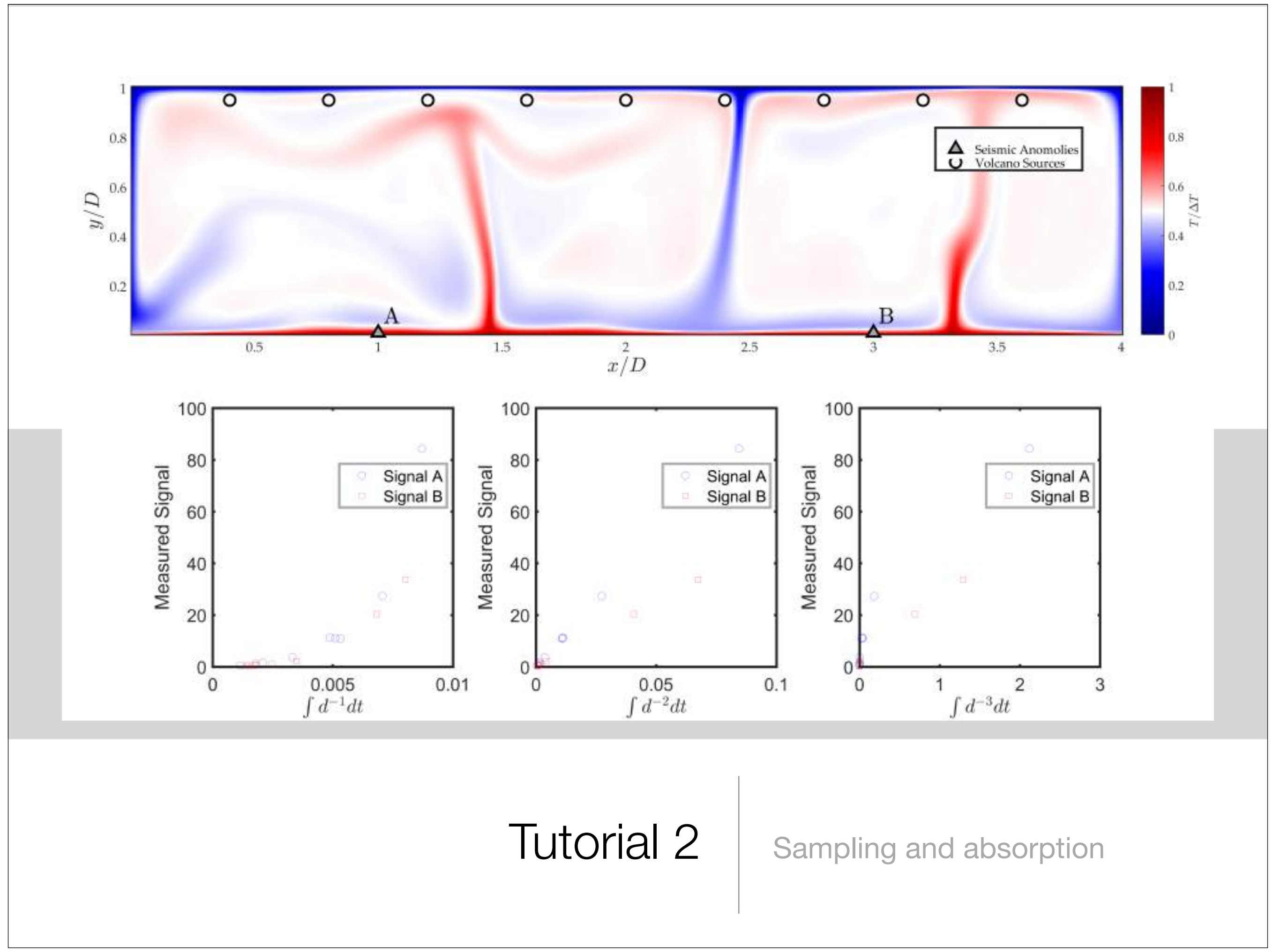
How might we use FTLE and LCS



[*Labrosse et al.*, 2015]

Origin of Heterogeneity

Genesis:
- -Primordial
- -Via Convection/Plate Tectonics



We assume that material absorbs a 'A' signal according to one of the three following models:

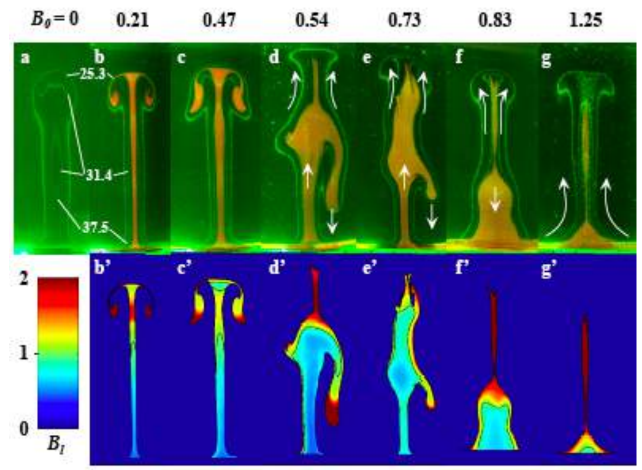
(1) d C_A /dt = r_A / d_A(t)
(2) d C_A /dt = r_A / d _A ^2(t)
(3) d C_A /dt = r_A / d _A ^3(t)

where d C_A / dt is the rate of change of the 'A' component of the geochemical signal, r_A is the rate of absorption of the 'A' signal, and d_A (t) is the distance of a fluid element from Source A. The equivalent models hold for Source B.

The participants are asked to identify which model is correct, and estimate the absorption rates (r_A and r_B), which are not the necessarily equal.

To do this, they have use different functions provided, including getinfo.m, which returns the previous trajectory of a tracer starting at a given location (x_o,y_o) that the user inputs, and writedataexcel.m, which converts the output of getinfo.m into an Excel spreadsheet with headers.

Active heterogeneity
density differences influences velocity field
(and, of course, amount entrained)

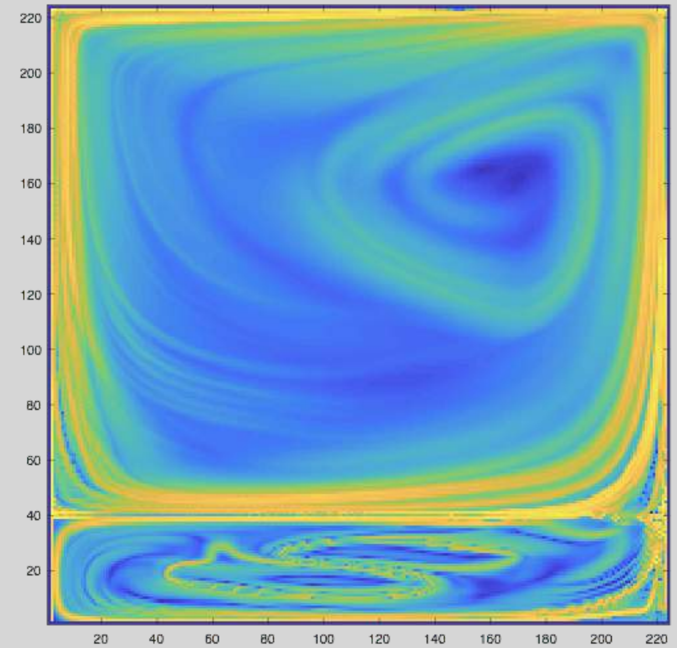


$$B_0 = \Delta\rho_{Xeff}/\rho\alpha\Delta T_{eff}$$

Kumagai et al., *GRL* 2008

Effects of composition

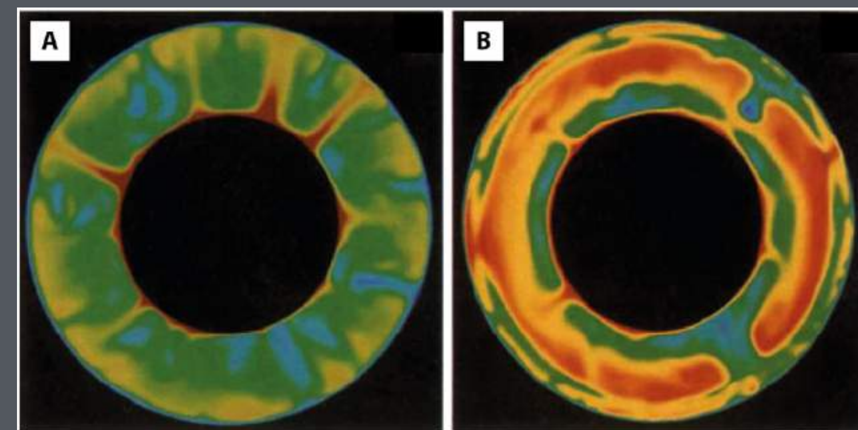
affects entrainment and mixing



220
200
180
160
140
120
100
80
60
40
20
20
40
60
80
100
120
140
160
180
200
220

FTLE field

Layered Convection



[*Tackley et al.*, 1993]

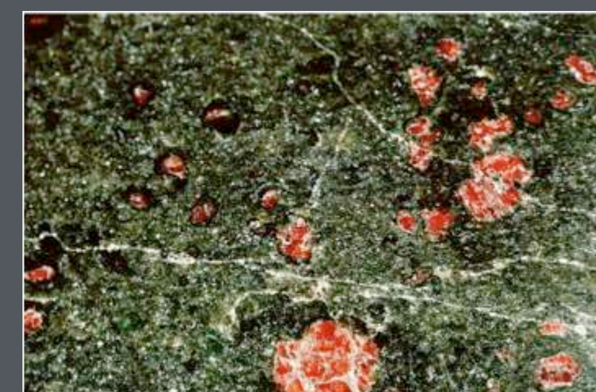
Demonstration of shutting off convection

Phase Transitions

$$
\begin{aligned}
\rho C_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) - \nabla \cdot k \nabla T = \rho H & \\
& + 2\eta \left(\varepsilon(\mathbf{u}) - \frac{1}{3}(\nabla \cdot \mathbf{u})\mathbf{1} \right) : \left(\varepsilon(\mathbf{u}) - \frac{1}{3}(\nabla \cdot \mathbf{u})\mathbf{1} \right) \\
& + \alpha T \left(\mathbf{u} \cdot \nabla p \right) \\
& + \rho T \Delta S \left(\frac{\partial X}{\partial t} + \mathbf{u} \cdot \nabla X \right)
\end{aligned}
$$

- Material Properties
- Thermodynamics (Static Properties)

Many Phases

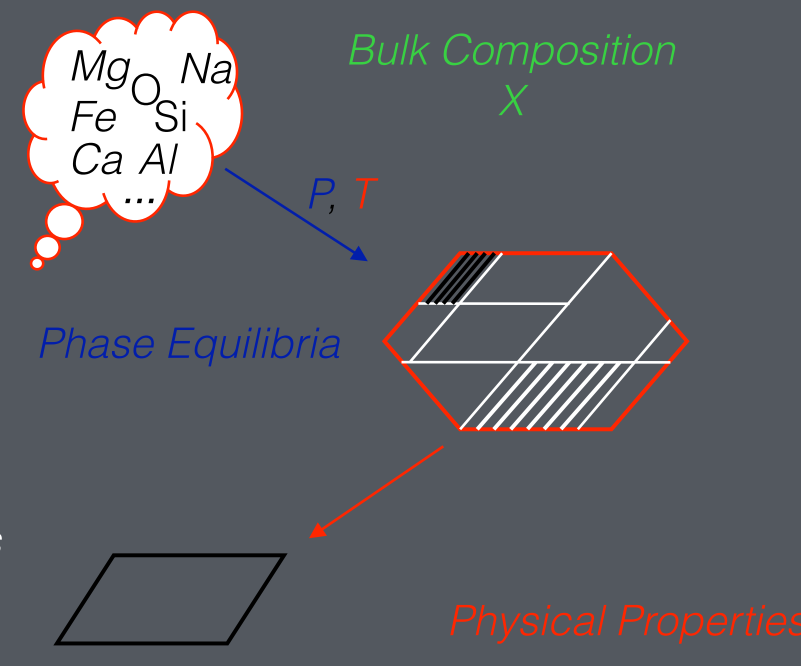


- *Equilibrium thermodynamics of multi-component systems*
- *Differentiation*
- *Affects physical properties*

Thermodynamic Model

- *Bulk composition*
- *Pressure*
- *Temperature*

- *Phase Equilibria*
- *Physical Properties*
- *Self consistent*



$\rho, \alpha, C_P, V_P, V_S, \ldots$ (X, P, T)

[*Stixrude and Lithgow-Bertelloni*, 2005; 2011]

HeFESTo

- *Based on Fundamental Thermodynamic Relations*
- *Minimize Gibbs free energy over the amounts of all species n_i*

$$G(P,T,n_i) = \sum_{i=1}^{species} n_i \left[\mu_{0i}(P,T) + RT \ln a_i\right]$$

- *Subject to constraint of fixed bulk composition*

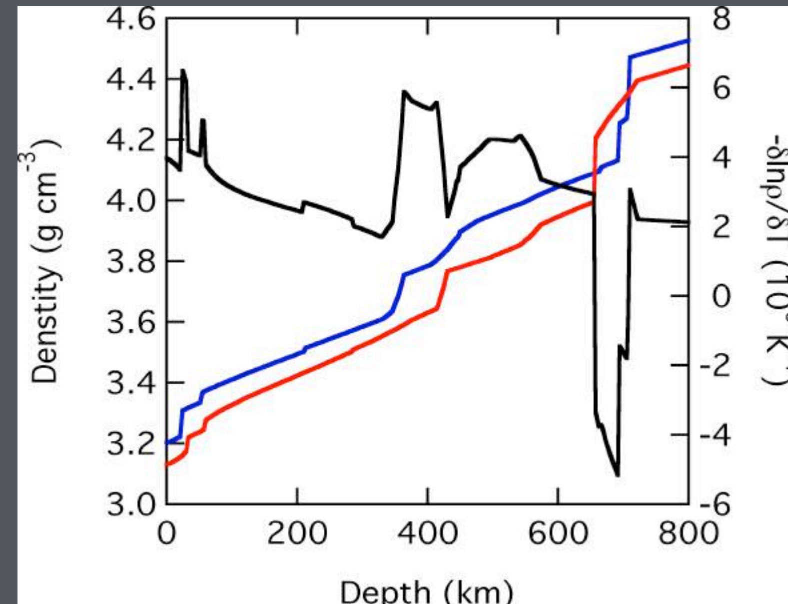
$$s_{ij} n_j = b_i$$

- *Full Anisotropic Generalization*

$$c_{ijkl} = \frac{1}{V}\left(\frac{\partial^2 F}{\partial E_{ij}\partial E_{kl}}\right)_{S'_{ij},T} + P\left(\delta_{ij}\delta_{kl} + \delta_{il}\delta_{jk} + \delta_{jl}\delta_{ik}\right)$$

- *Many previous efforts, however*
  - *Full self-consistency between phase equilibria and physical properties (not only one or the other)*
  - *Anisotropic generalization and robust thermal extrapolation for shear properties*

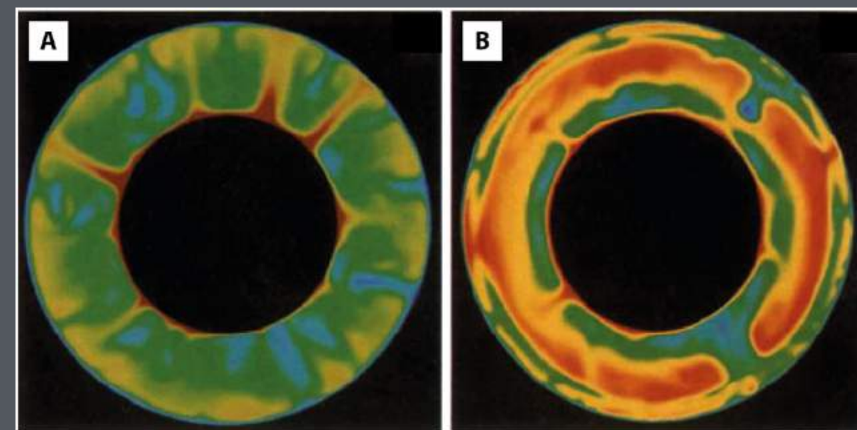
Phase Transitions and Convection



[*Stixrude and Lithgow-Bertelloni*, 2007]

Self consistent calculation of physical properties and phase equilibria and here it's what happens. Here is a cold adiabat in blue and a hot adiabat in red and mostly density decreases on heating, but here because of the phase transitions they are crossing in the wrong direction, and this negative thermal expansion shuts off convection.

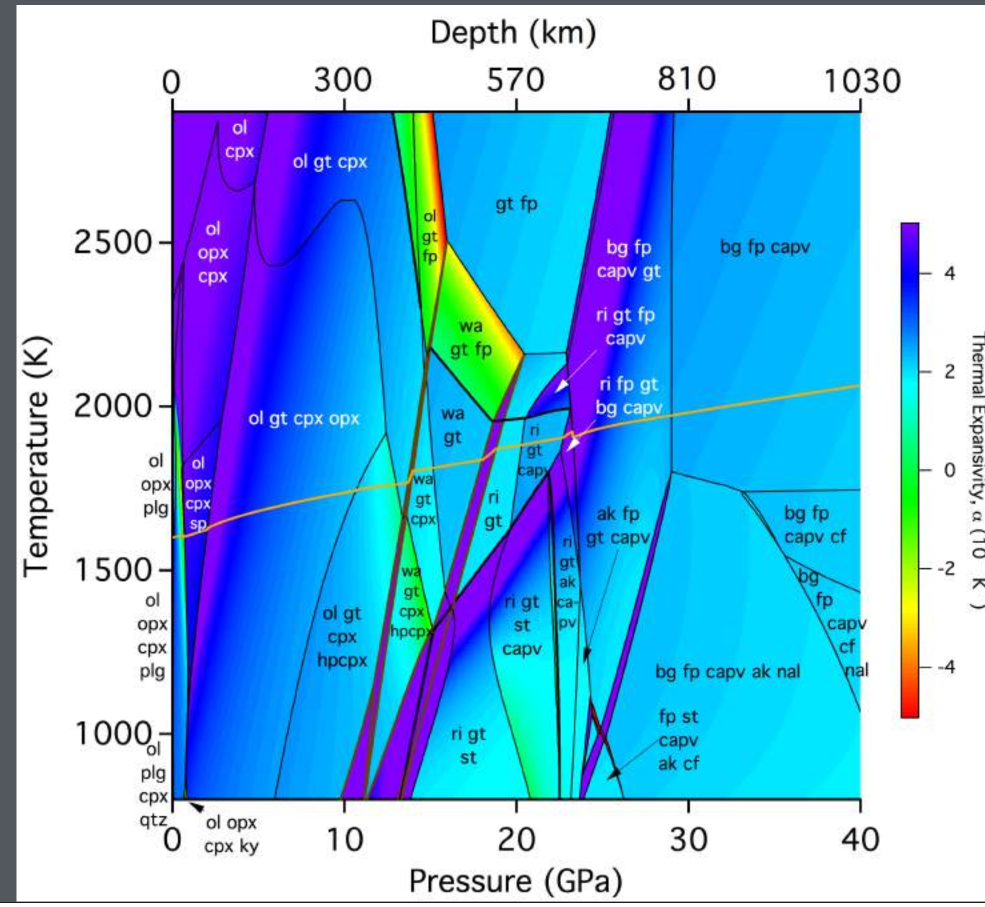
Layered Convection



[*Tackley et al.*, 1993]

Demonstration of shutting off convection

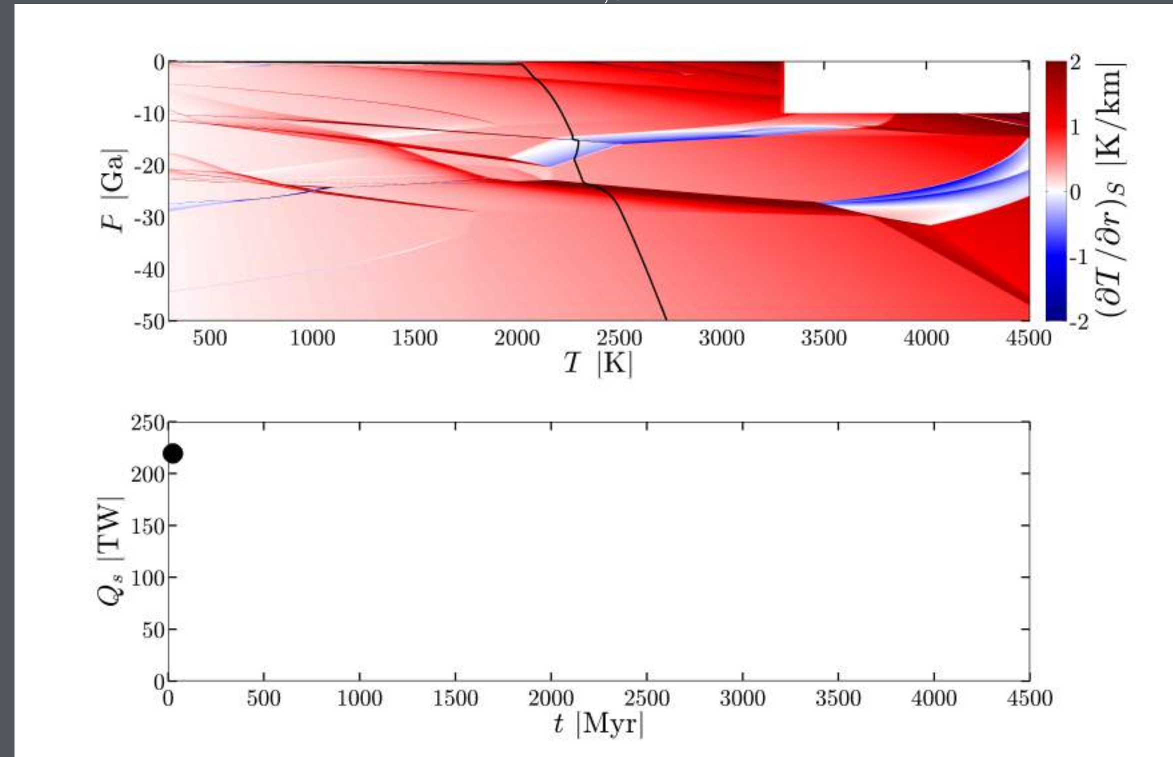
Physical properties



What about other geotherms in the past, look at it in a different way, look at all the negative thermal expansion.

EVOLUTION

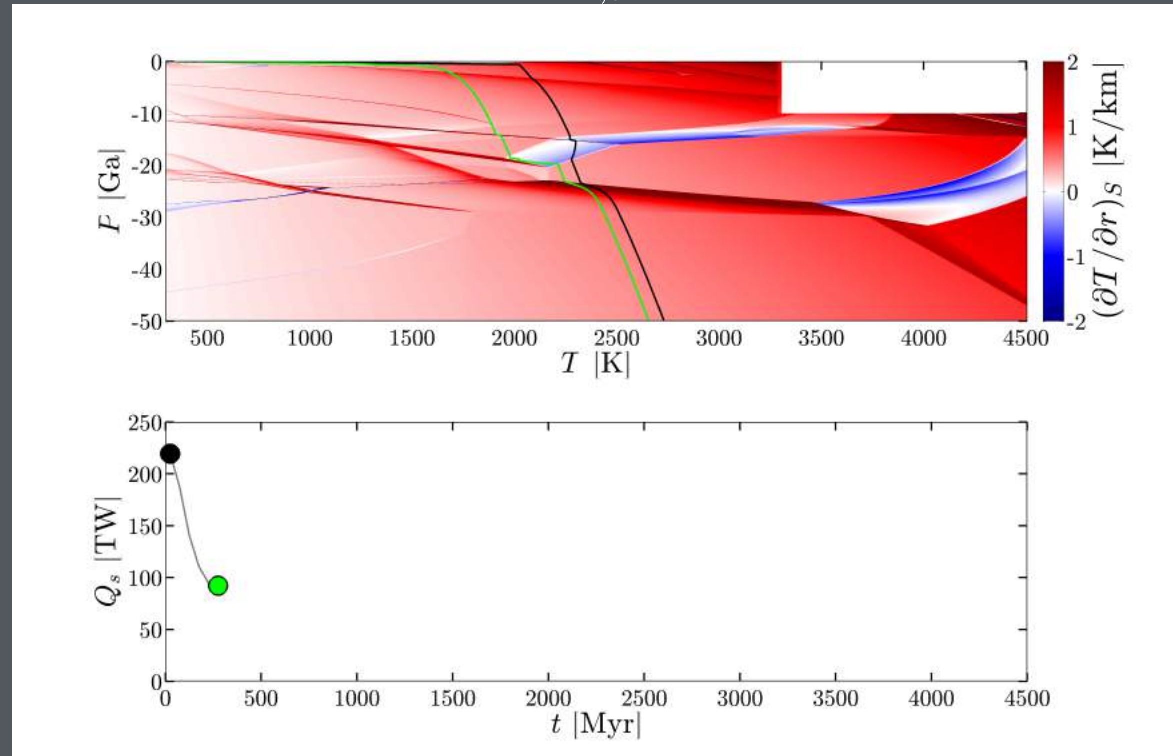
Initial $T_{P,0}$=2000 K



Geotherm at t=0 passes through region of negative $\boldsymbol{\alpha}$

EVOLUTION

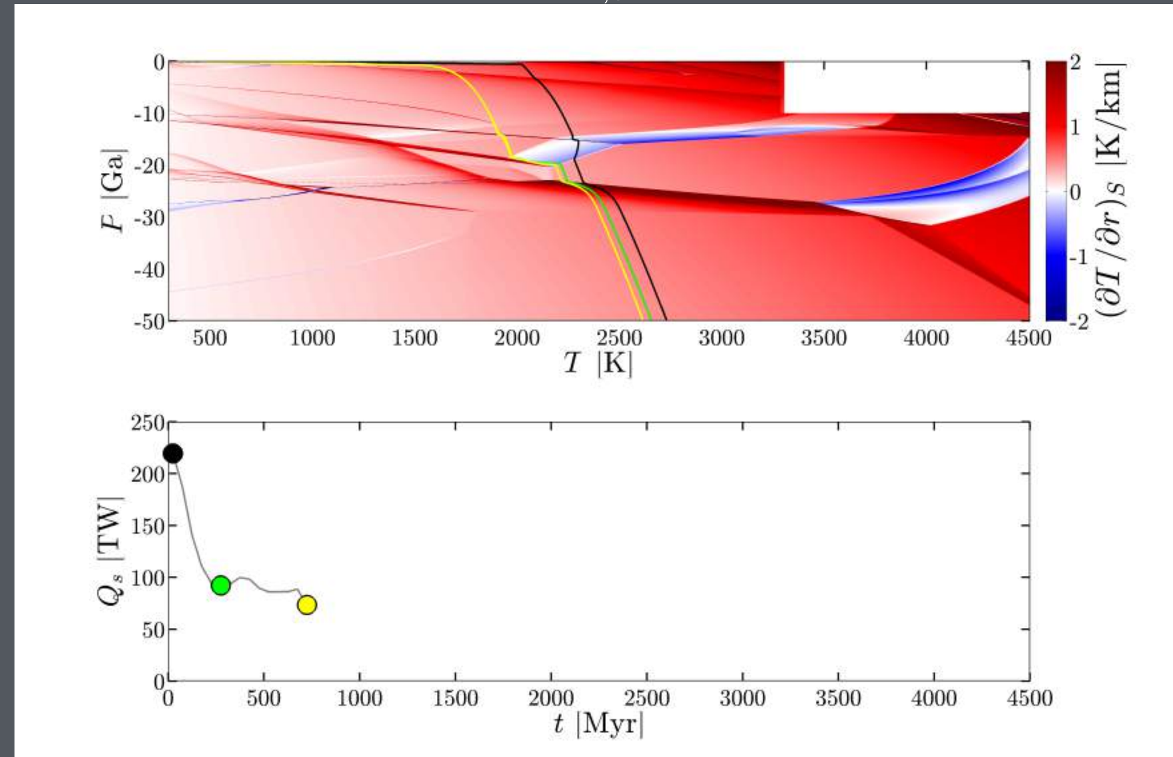
Initial $T_{P,0}$=2000 K



Shallow mantle rapidly cools

EVOLUTION

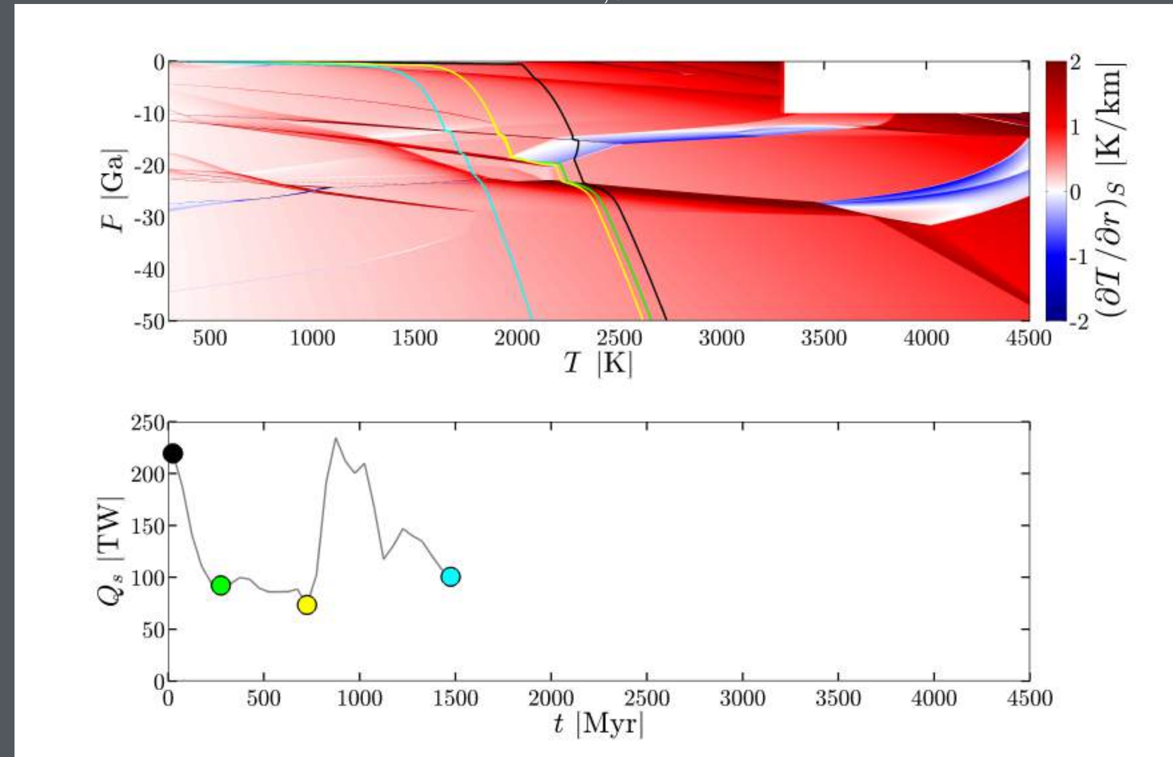
Initial $T_{P,0}$=2000 K



Rising T causes α to become negative-Lower mantle is insulated

EVOLUTION

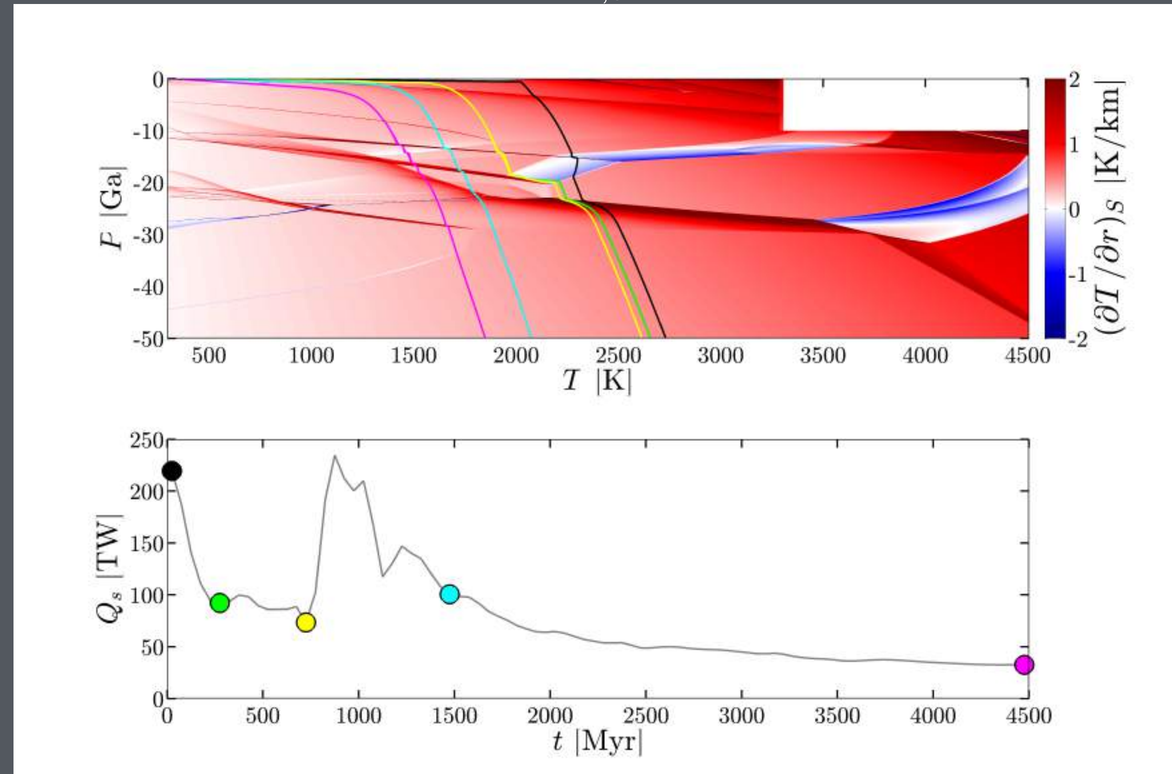
Initial $T_{P,0}$=2000 K



Once geotherm can bypass this region-heatflow is rapid

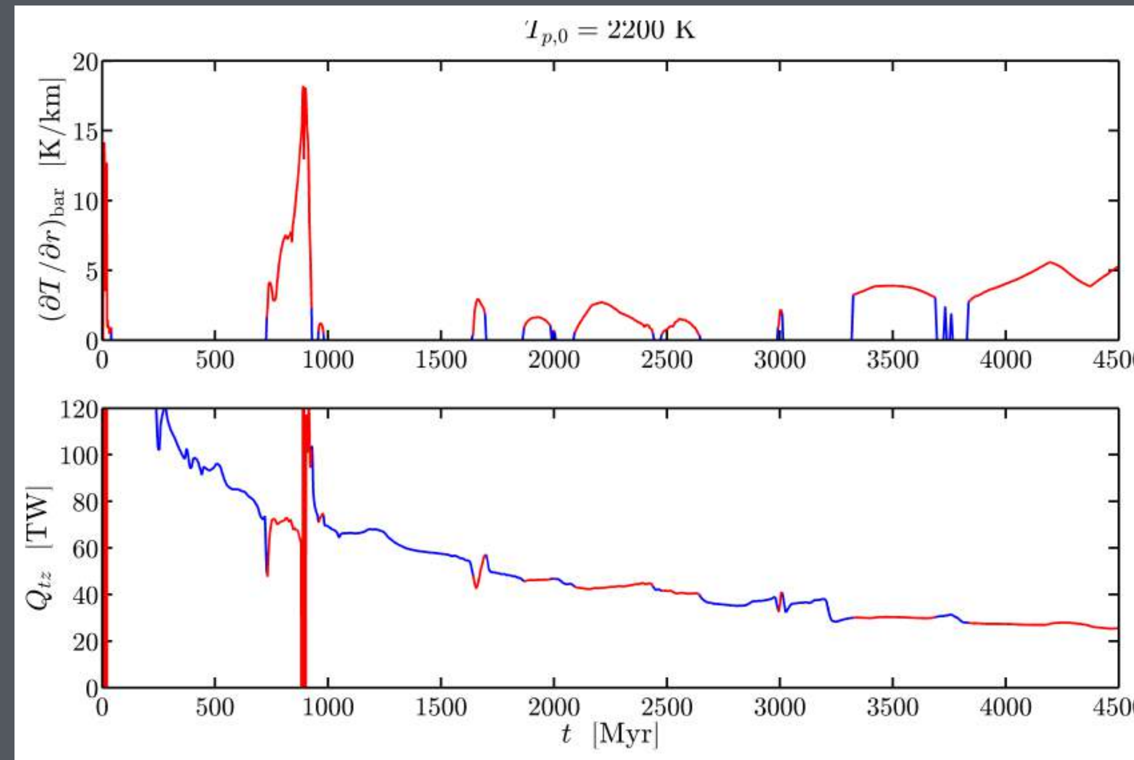
EVOLUTION

Initial $T_{P,0}$=2000 K



Roughly steady after this point (including present-day)

Intermittent Layering



- *Layered state about ~80% of the time*