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The iron spin transition

Identification and implications for mantle dynamics

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The iron spin transition

Identification and implications for mantle dynamics





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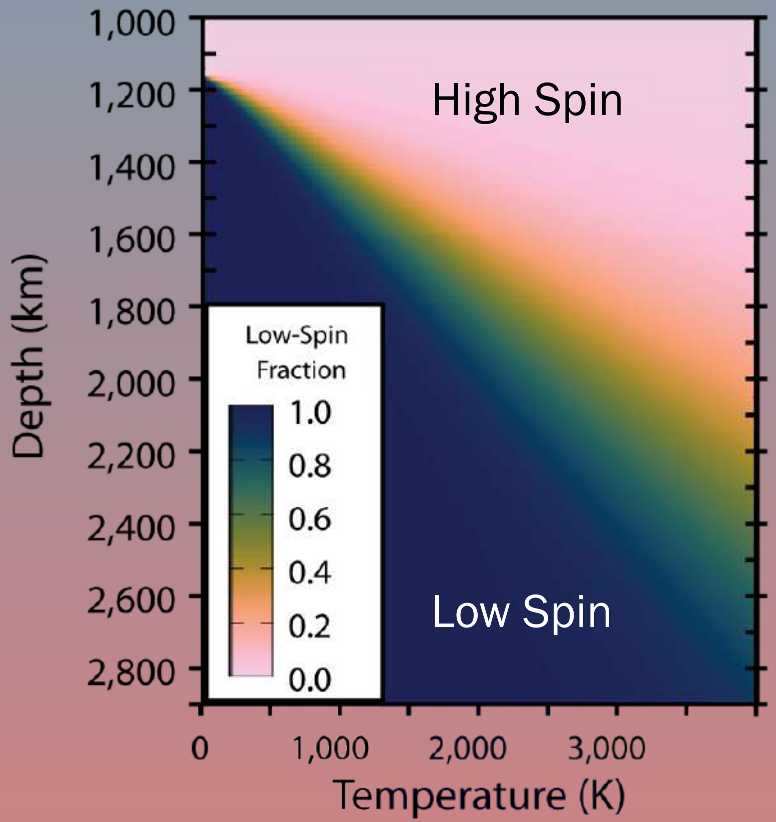
Aim of this study

- Ferropericlase ~20% lower mantle
- Iron in Fp undergoes a spin transition
- Experimentally proven but not readily apparent in seismic data



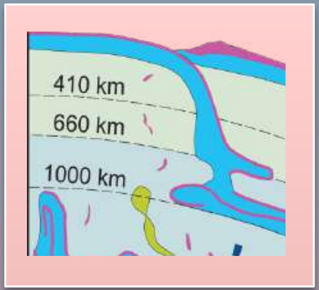
Why not

Are mineral physics predictions wrong ?
Seismic resolution poor ?
Is there not enough Fp?

Aim of this study

Spin changes thermo-elastic properties and convective behaviour:

- Slabs
  May stall, reorganise or avalanche
  (e.g. Morra et al. 2010, Shahnas et al., 2011)



- Plumes
  May enhance vigour, plume head dynamics
  (e.g. Bower et al., 2009; Shahnas et al., 2011; Justo et al., 2015)

- LLSVPs
  May enhance boundaries and stability, or not.
  (e.g. Huang et al. 2015; Li et al., 2018)

Talk Overview

[1] Overview Mantle Structure and Composition

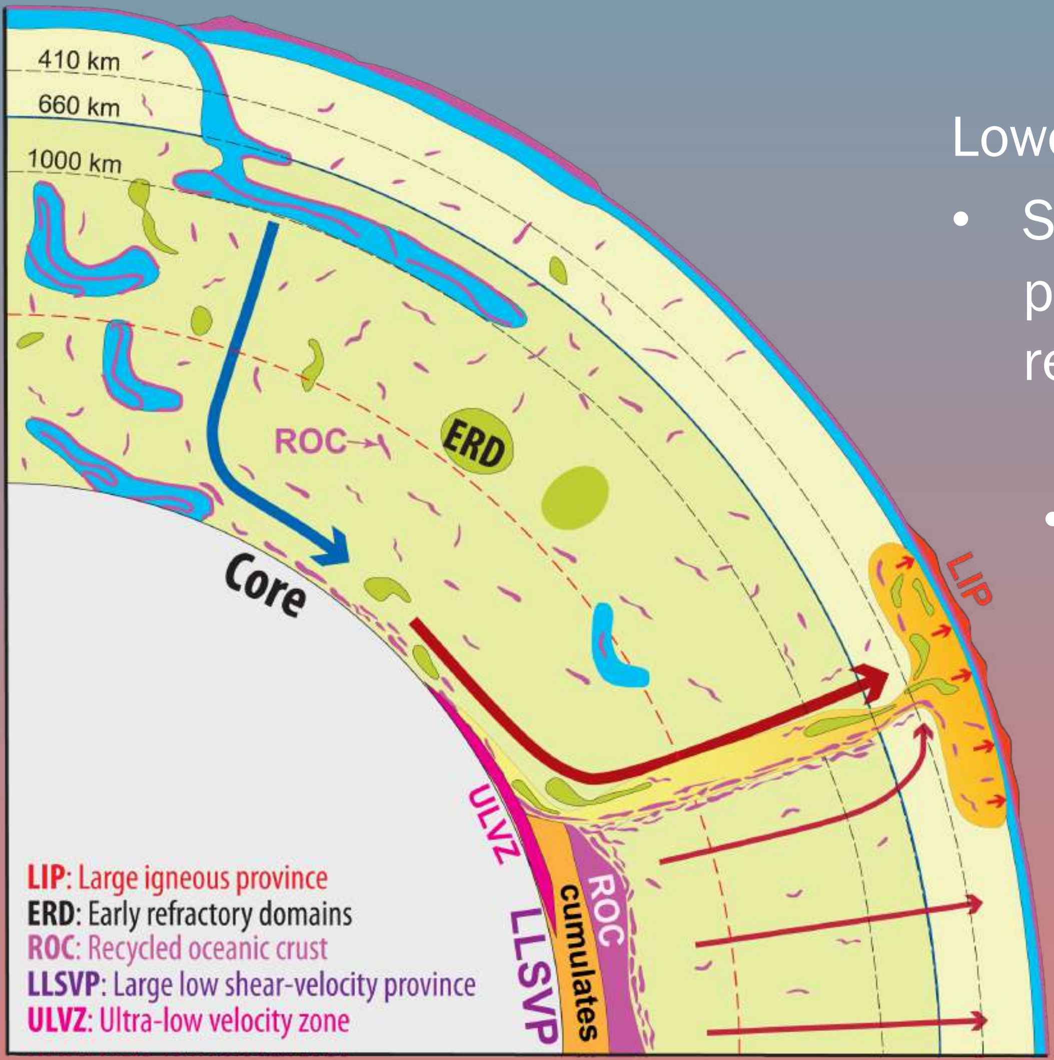
[2] Iron spin transition
- Mineral physics
- Seismology

[3] Vote maps

[4] Geodynamic implications
- BEAMS structures

Mantle structure and composition

Structure of the mantle



Lower mantle:

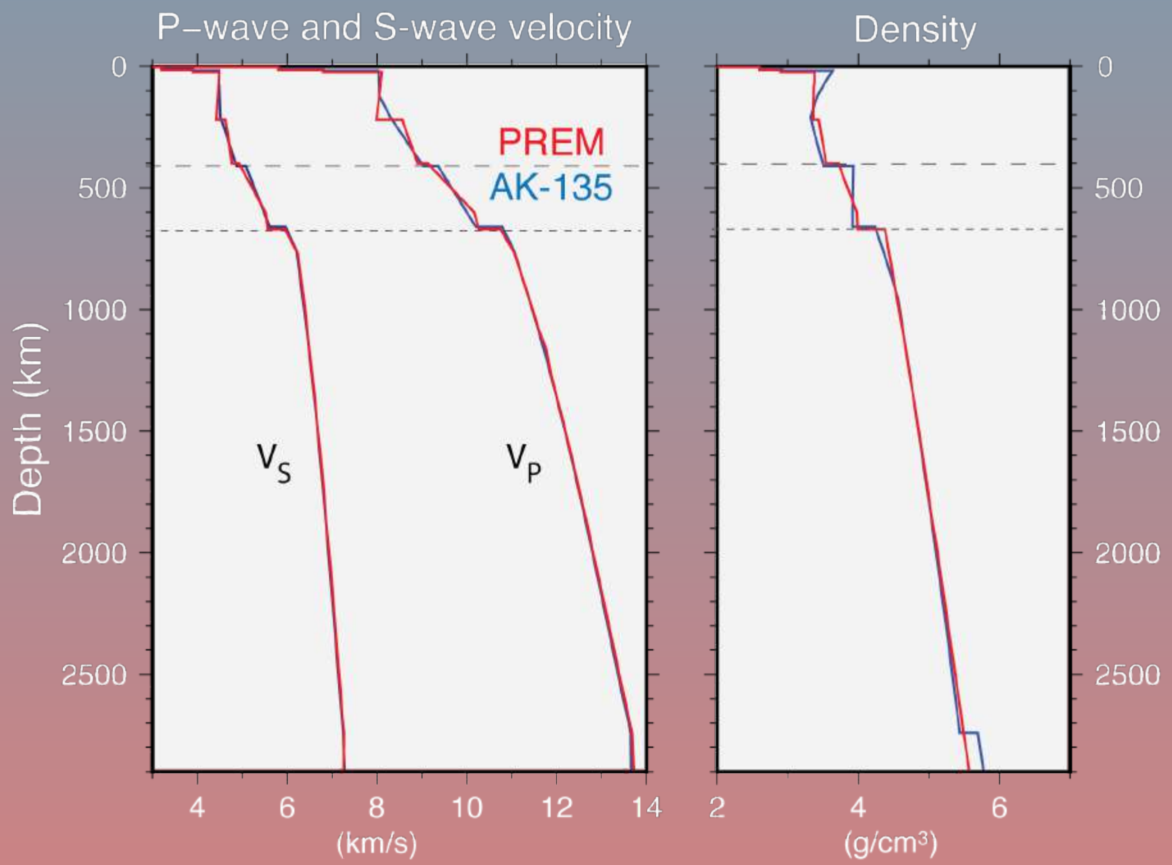
- Subducted slabs, mantle plumes, LLSVPs, ULVZs, recycled and primitive features
  - Mixing/mass transfer with upper mantle
    - Variable modes of convection

Reidar Trønnes: Trønnes (2010), Torsvik et al. (2016)

Structure of the mantle

Standard 1-D radial density and velocity models

- ‘First order’ phase changes leading to reflections
- Not within the lower mantle



References: Dziewonski et al. (1981); Kennett et al., (1995)

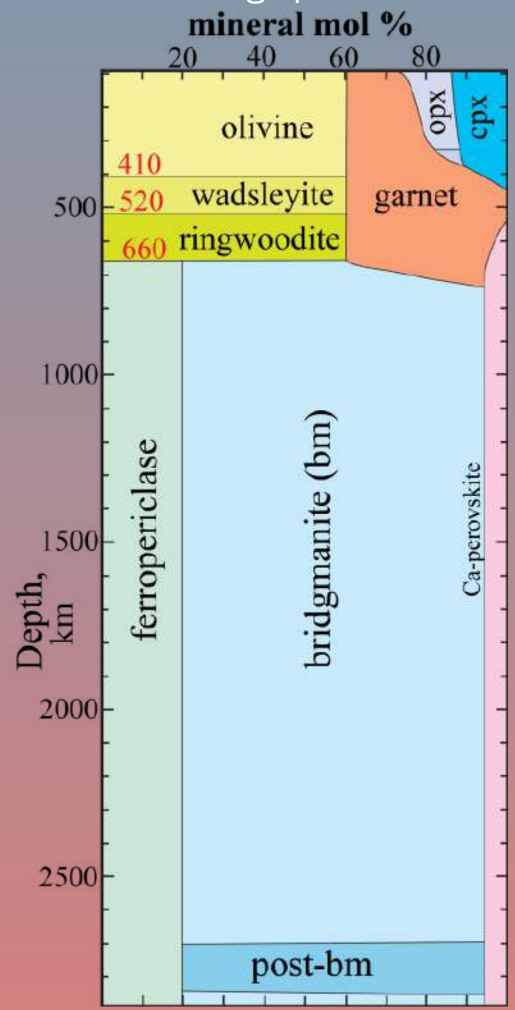
Composition of the mantle

Thought to be a pyrolite and if similar to upper mantle (Mg/Si ratio ~1.27):

- 80% (Mg,Fe)SiO_3 bridgmanite
- 20% (Mg,Fe)O ferropericlase
- Minor $CaSiO_3$ Ca-perovskite (also ppv)

- Mg/Si, Mg/Fe, Ca/Al ratios an outstanding question, as well as Fe partitioning

Average peridotite



Reidar Trønnes

Composition of the mantle

Bridgmanitic – Pyrolitic – Harzburgitic

Si rich(er)
Bm rich, Fp poor(er)
Imply distinct UM/LM
Rheologically stronger
(Mg+Fe)/(Si-Ca) ~ 1

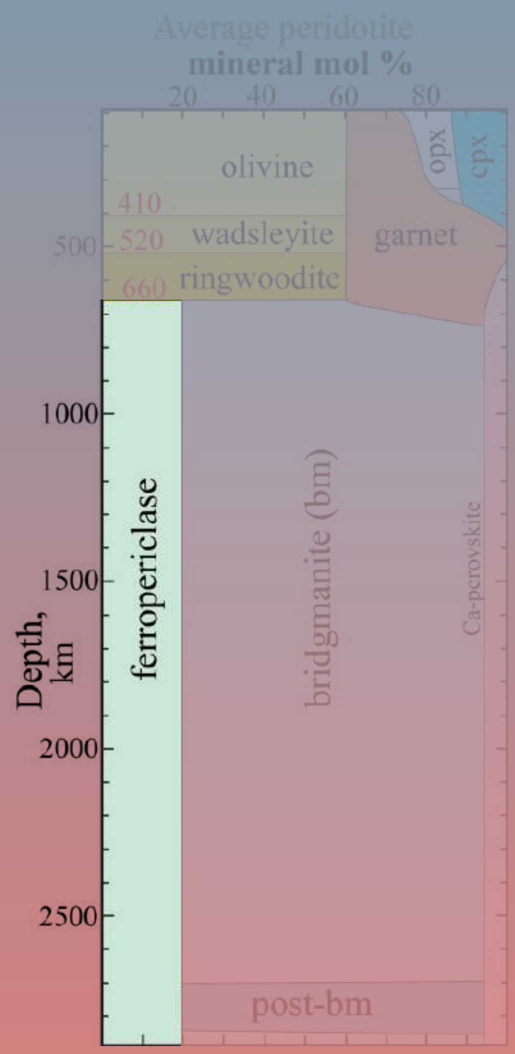
Si poor(er)
Fp rich(er)
Implies mixing
Rheologically variable
(Mg+Fe)/(Si-Ca) > 1

Predicted seismic responses of different compositions greatly affected by temperature therefore not readily discriminated

Composition of the mantle

<u>Ferropericlase</u> (Mg,Fe)O

- A major host for iron in the lower mantle
- Fp requires (Mg+Fe)/(Si-Ca)>1
  i.e. olivine in addition to pyroxene
- Ferrous iron (Fe^{2+}) cation undergoes electronic transition which affects elastic properties and therefore seismic response
  - Opportunity to constrain composition

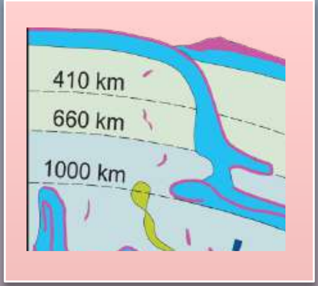


So where to look for Fp?

- Slabs…

  Fp-rich: 7% basalt and 93% depleted harzburgite

  Si-depleted, ~23% Fp



- Plumes…

  recycled component, might also contain other Si-rich entrained components

- Ambient…

  possibly the least Fp

Things to disentangle (keep in mind)

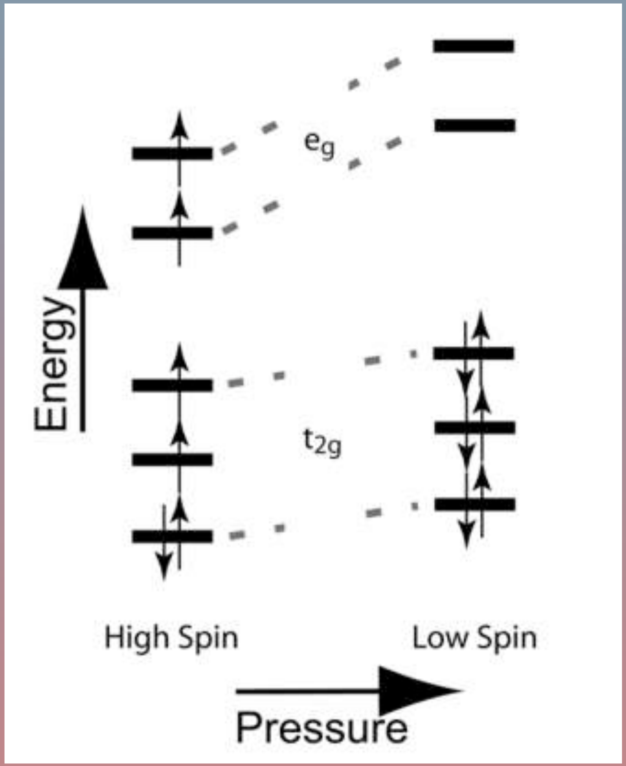
Untangling relatively subtle signals caused by overlapping and/or unconstrained effects:

- Uncertainties in LM material properties, T and composition
- Effects on seismic velocities
- Other mid-mantle changes e.g. viscosity/density change
- Changes in subduction flux
- Influence from pPv and LLSVPs
- Plus others…

Iron Spin Transition

Iron Spin Transition

- First proposed by Fyfe (1960)
- Spin transition = pressure induced rearrangement of electrons and energy of chemical bonds ("spin pairing")
- Collapse of electron orbitals of iron (3d) from high to low spin state
  - Mixed spin/spin transition
- Reduces cation size (volume) changing physical properties of Fp



Speziale et al., 2005

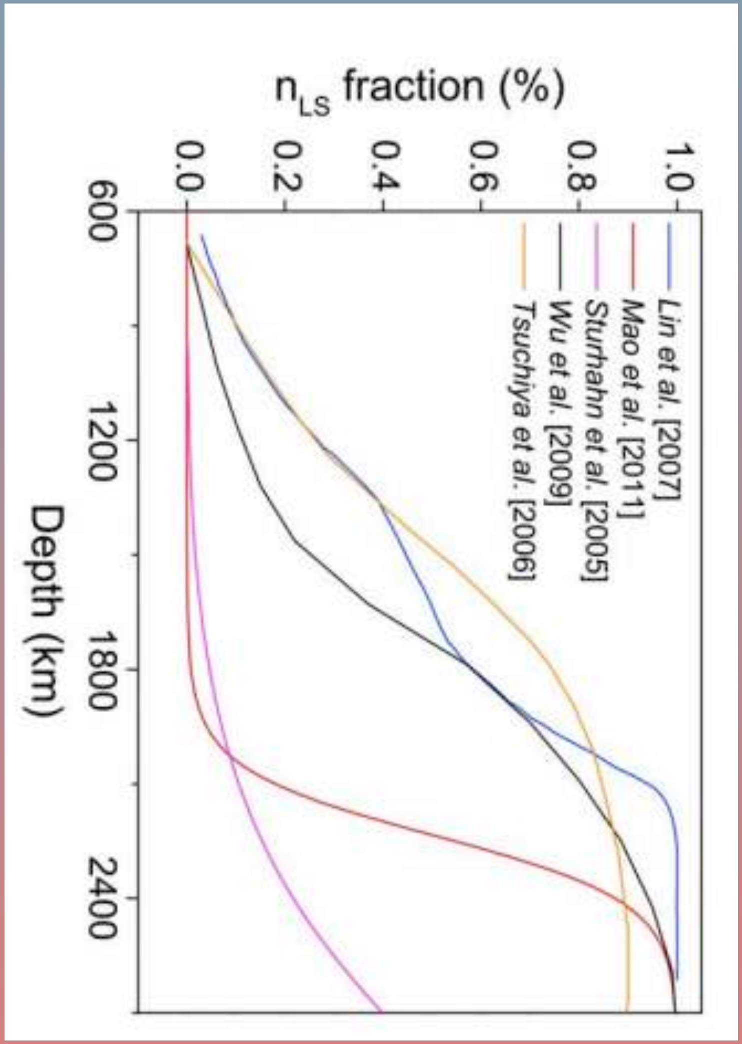
Iron Spin Transition

- Experimentally confirmed by Badro et al. (2003)

  ~60-70 GPa
  ~1000-2200 km depth
  ~1900-2300 K

  – Broad (unlike ordinary phase transitions)

- P-induced but also affected by mantle T and composition, and Fp composition and abundance



Lin et al. (2013)

References: Lin et al., 2005; Wu and Wentzkovitch 2015

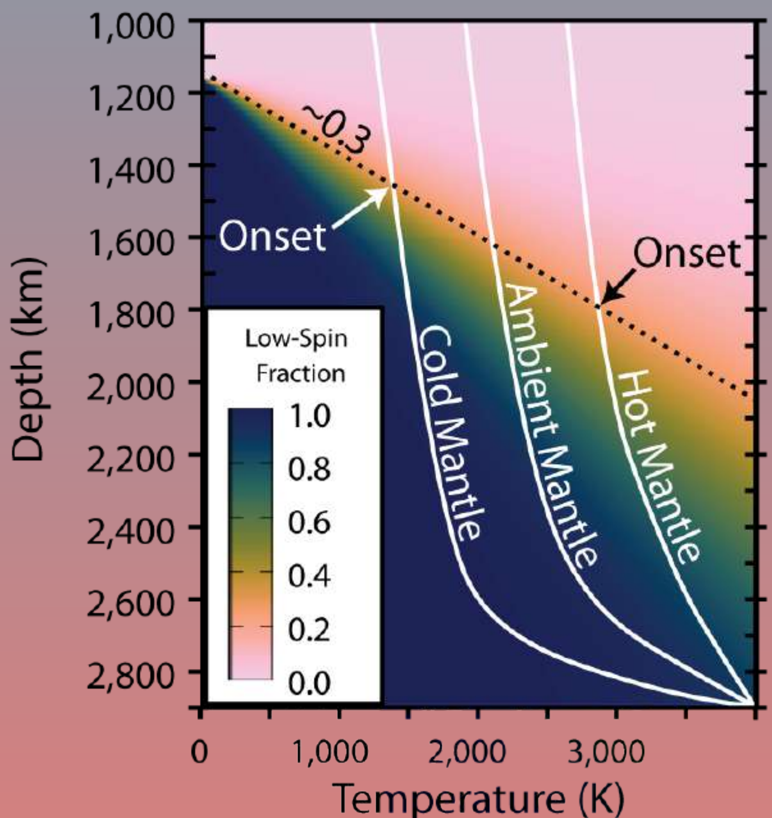
Iron Spin Transition

Fe concentration of x=18.75% in FpMg(1-x)FexO

$$n_{LS} = \frac{1}{1 + \exp(\Delta G(P, T)^* / T)}$$

Promoted by increasing pressure and decreasing temperature:

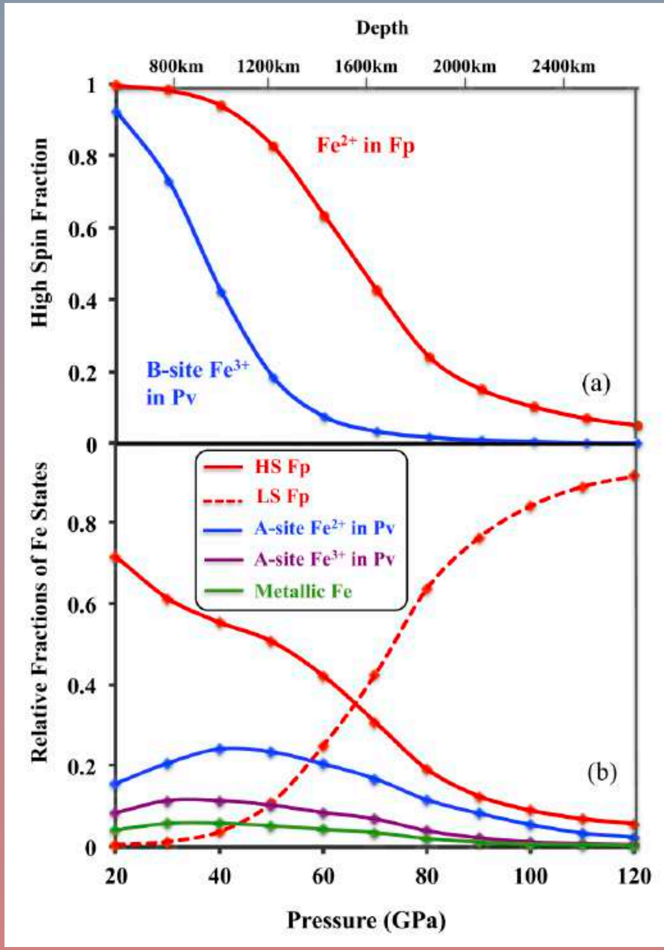
- Increasing width of the mixed phase region
- Cold geotherm: ~1400 km onset
- Hot geotherm: ~1700 km onset.
- Possible presence of mixed spin to CMB



Shephard et al. (in prep)

FAQ: Why not in Bridgmanite?

- Different crystallographic and oxidation states.
- Role of Al (Fe^{+2}→Fe^{+3})
- Iron is part of Fp backbone, but not for Bm (SiO_6 octahedra are most important structural framework for Bm).



Xu et al. (2016)

References: Lundin et al. (2008); Lin et al. (2008)

Iron Spin Transition

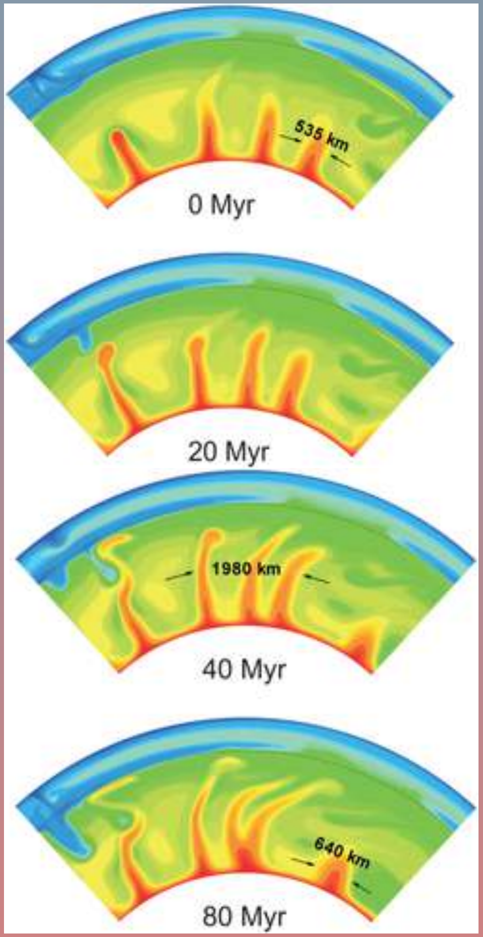
Effects:

Significant effect on density (~1%)

Bulk modulus softens (!)

Little effect on shear modulus

- Changes in viscosity, radiative thermal conductivity, thermal expansion, heat capacity and creep activation parameters, enhancement of anisotropy, convective vigour etc.
- Changes iron partitioning and speciation (suppresses Fe^{3+} and metallic Fe formation)



Shahnas et al. (2016)

(K) Bulk modulus

Hulk Modulus

The ratio of the increase in pressure to resulting fractional change in volume

$$K = -V\frac{dP}{dV}$$

- i.e. the compressibility of the material
- Volume change requires bulk modulus change (!)
- Dramatically softens during the spin cross-over
  - E.g. by ~250 GPa at 300 K for x =0.1875 (Wu et al., 2013)

Spin’s seismic expectations

Seismology basics

Mapping of travel time curves to seismic velocities

- P-wave (V_P): Compressional/Dilational
- S-wave (V_S): Shear/Rotational
- Velocities depend on physical properties of the material; elastic moduli and density

$$V_P = \sqrt{\frac{K + \frac{4}{3}\mu}{\rho}} \qquad V_S = \sqrt{\frac{\mu}{\rho}}$$

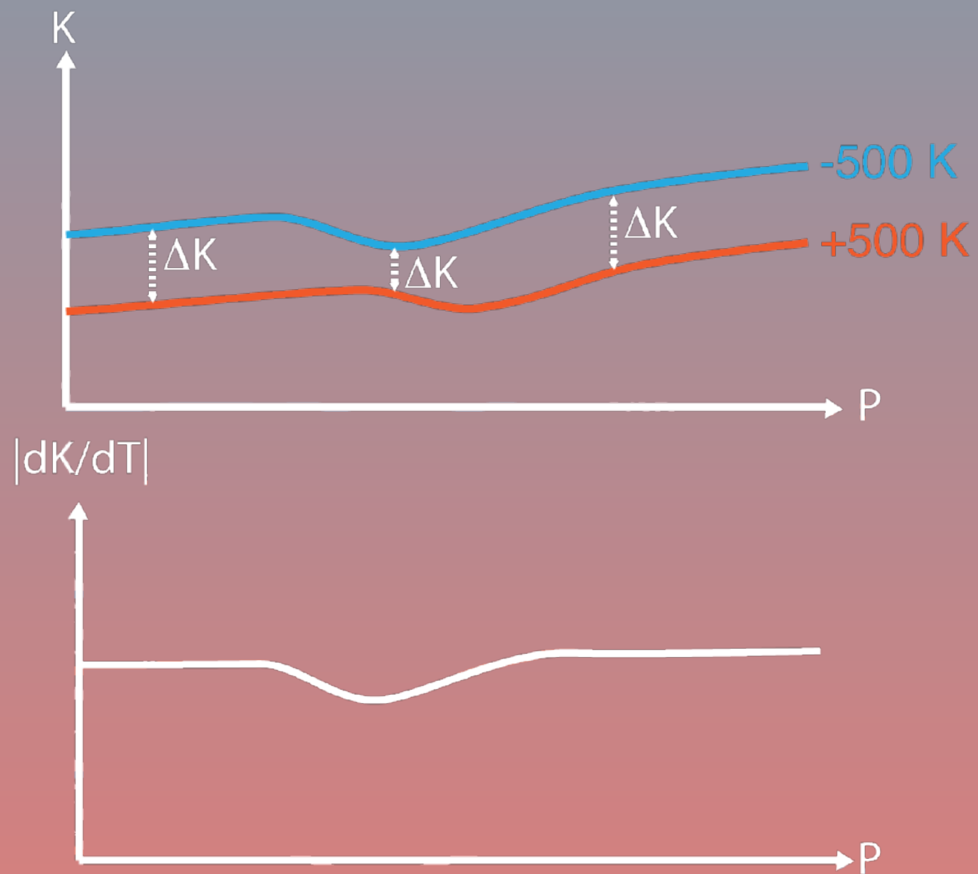
- Affected by temperature, pressure and composition

Spin's seismic predictions

Temperature:

In addition to shifting the pressure range of the spin transition

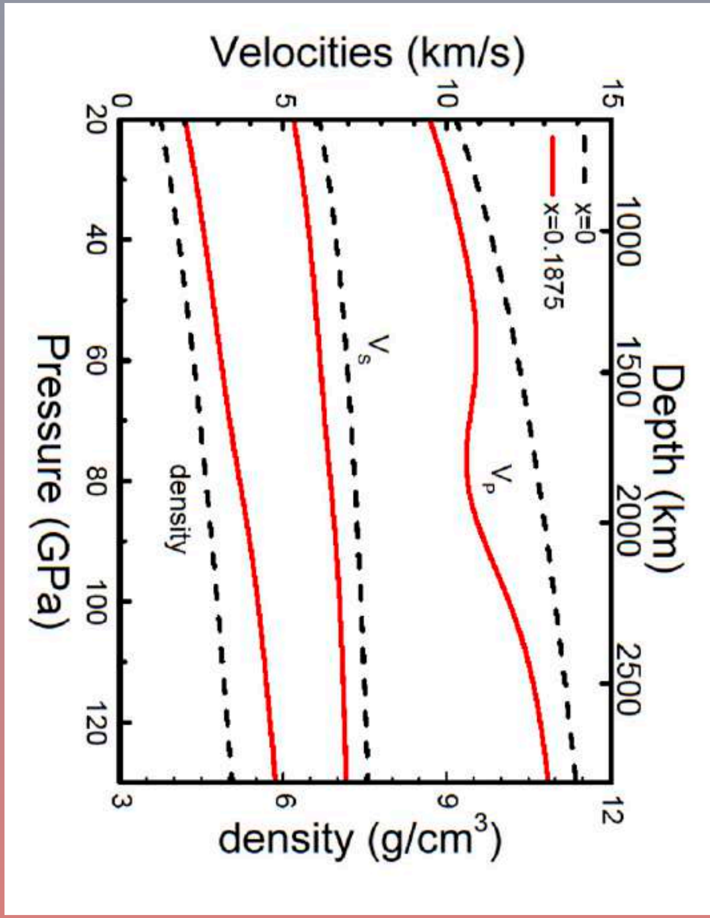
- Reduces sensitivity of V_P to lateral T variations



Spin's seismic predictions

Composition:

- Enhances sensitivity of V_P (and V_Φ) to composition
  - Increasing Fe/(Fe+Mg) decreases all velocities and enhances effect on V_P



Lin et al. (2013)

Spin's seismic predictions

In short:

- V_P expected to decrease in the transition
- V_S expected to stay the same

AND

- dV_P/dT decreases in the transition
- dV_S/dT expected to stay the same

Has it been seismically detected before?

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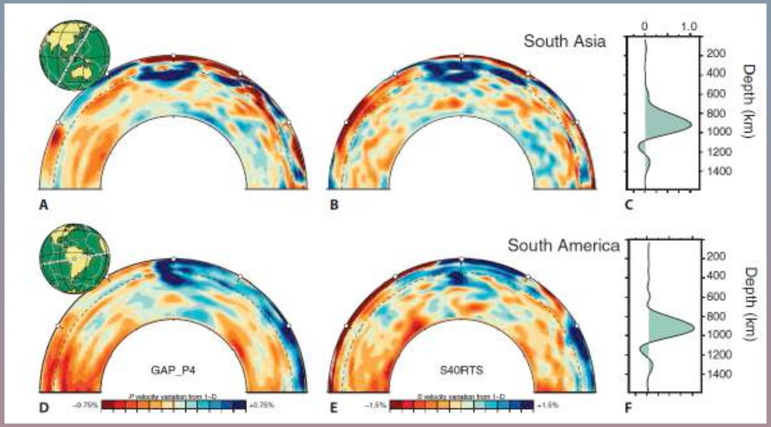
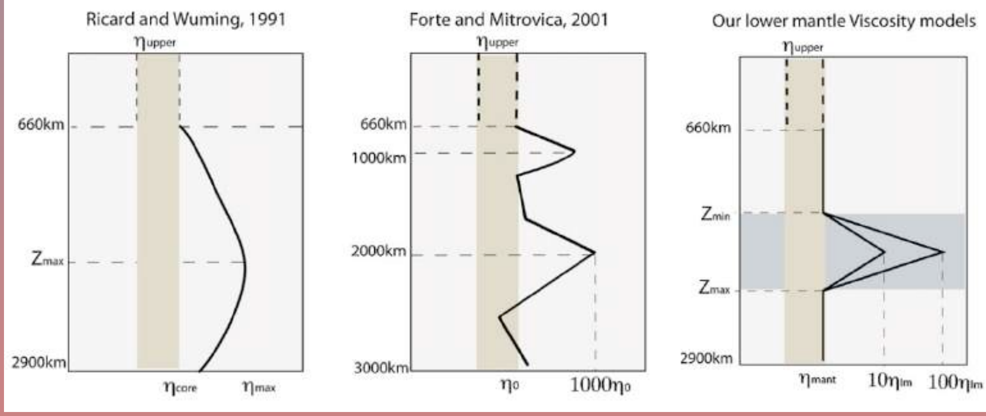
Something's going on:

- Slab stagnation and plume disruption
  - Mid-mantle viscosity/density variation?
  - Dense MORB, Bm-enriched, Bm-dewatering?



Ballmer et al., 2015



Morra et al., 2010

References: Zhao (2007); van der Hilst and Karason (1999); Wu and Wentzkovitch (2014) ; Boschi et al. (2007); Masters (2000) and many others

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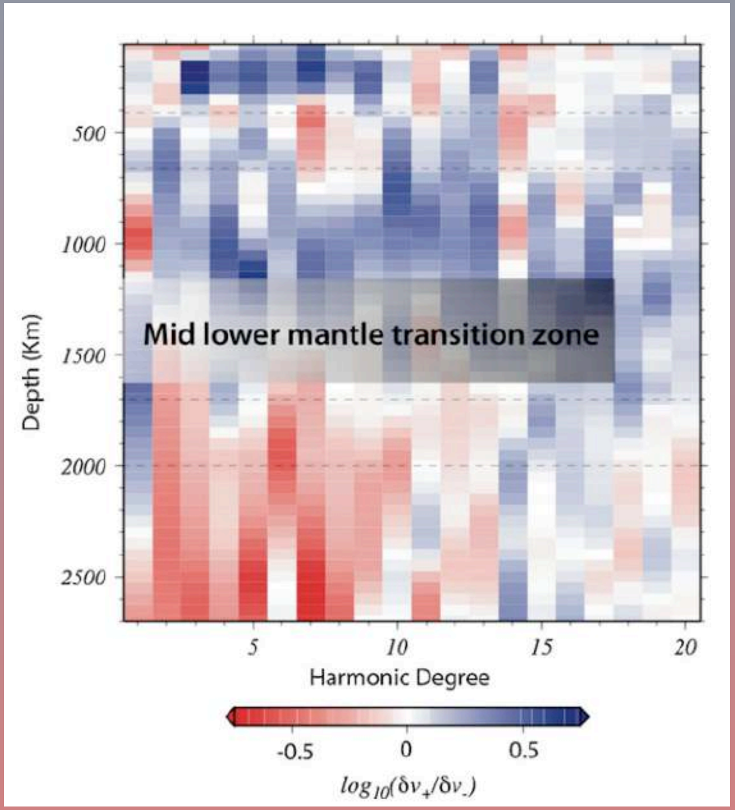
- Spectral changes
  - Anti-correlation of V_S and V_Φ

  Not necessarily compositional change
  - V_P-V_S ratios

Morra et al., 2010 from Boschi et al., 2010 (SMEAN)



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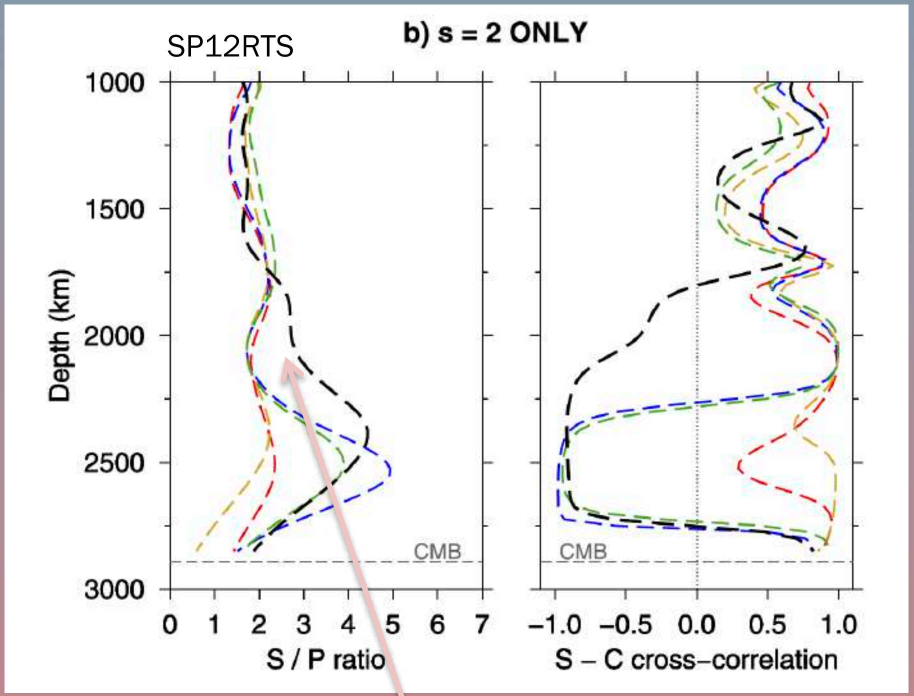


Koelemeijer et al. (2018)

References: Zhao (2007); van der Hilst and Karason (1999); Wu and Wentzkovitch (2014) ; Boschi et al. (2007); Masters (2000) and many others

Has it been seismically detected before?

The upshot: hinted at but not clearly shown…

FAQ: So what are we doing differently?

Here we look into

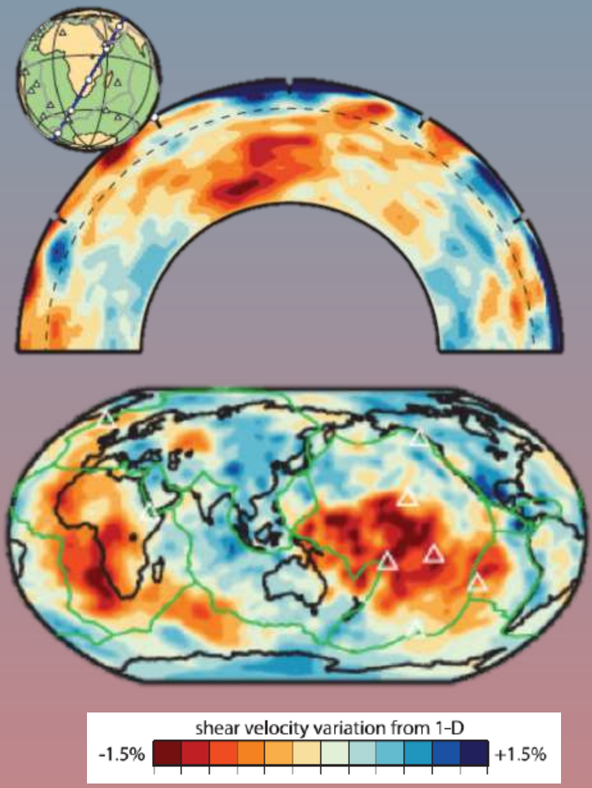
- V_P and V_S
  - fast, slow, and ambient domains
- Multiple tomography models
  - Avoiding those that are similar (e.g. joint inversions)
- Map out the behaviour laterally and radially
  - Quantified in terms of surface area per depth

Seismic tomography

Seismic tomography

- 3-D velocity structure of the Earth
  - Different seismic phases, methods and approximations
  - Body wave travel times, surface wave dispersion, normal modes

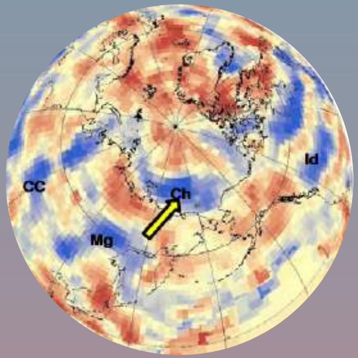
- General agreement on broad structure
  - High velocities = slabs (positive anomalies)
  - Low velocities = plumes, LLSVPs (negative anomalies)
  - Vp and Vs similar resolution in mid-mantle



Ritsema et al. (2011)
S40RTS

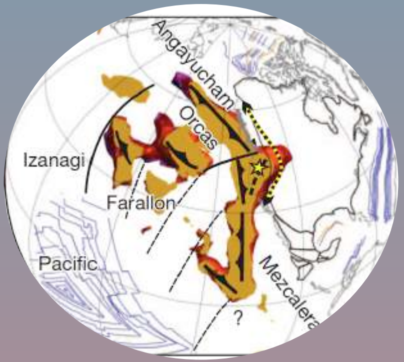
Linking surface and deep

Global, Regional, Absolute frame



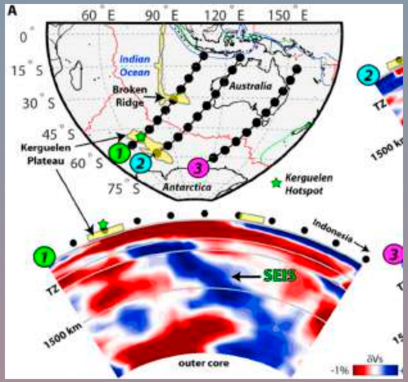
Van der Meer et al.
(2010; 2013; 2017)

Regional – Farallon



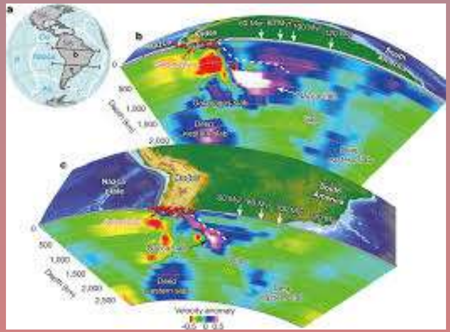
Sigloch and Mihalynuk, 2013

Regional – SE Indian



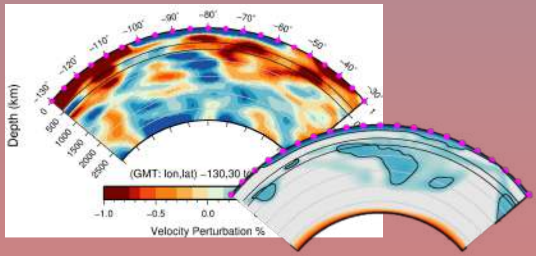
Simmons et al., 2015

Regional – South America

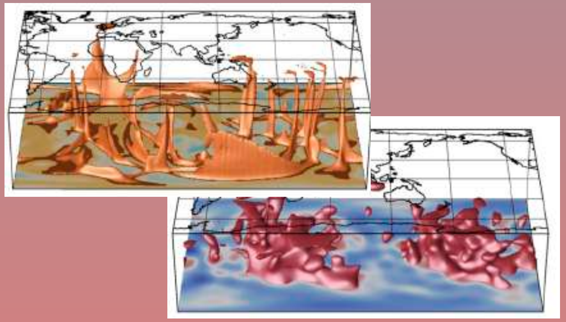


Chen et al., 2019

Numerical modelling



Shephard et al., 2014



Bull et al., 2009

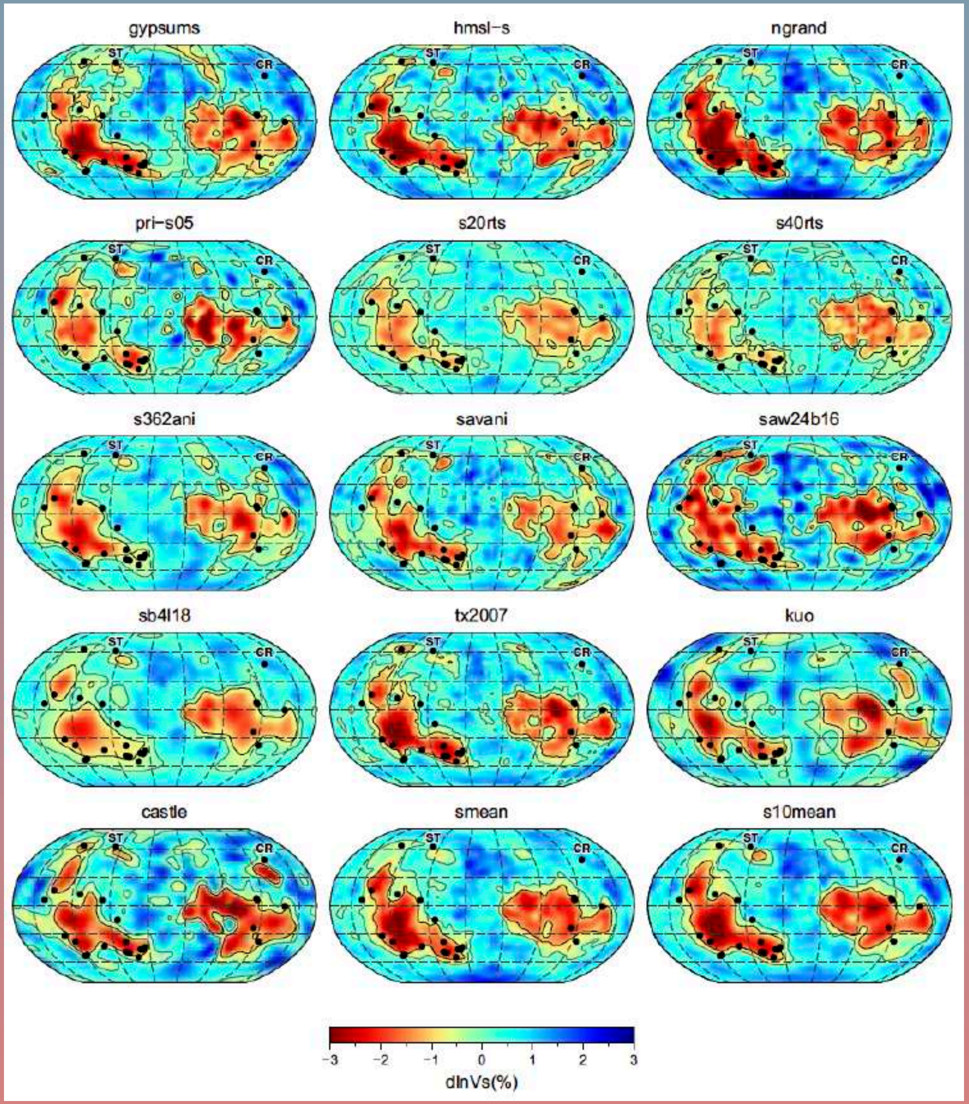
Seismic tomography

Broad spectrum of models to use

Can be difficult to assess resolution and 'reality' of a given model at a given depth/location

While a Vp/Vs anomaly might result from parameterization choices etc

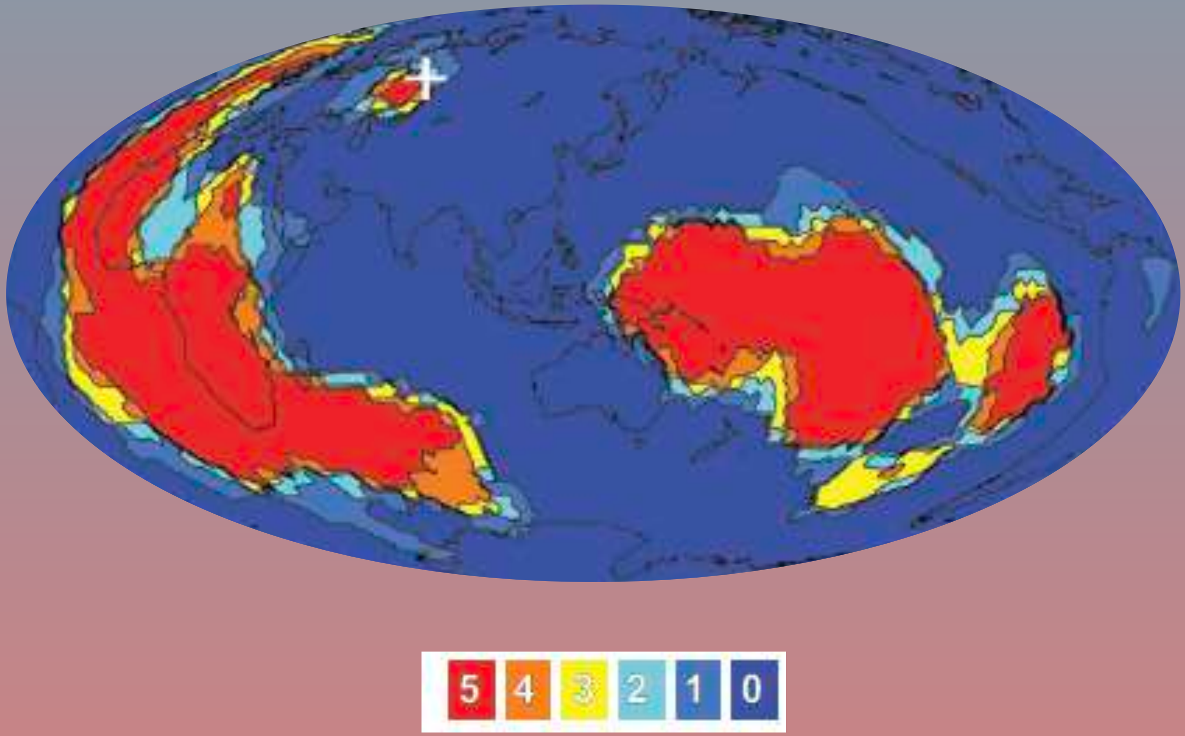
→ unlikely to persist across numerous models



Doubrovine et al., 2016

Seismic tomography

Basically, does a given blue blob really warrant being identified as a slab?



Lekic et al. 2012
Cottaar and Lekic, 2016

Vote map method

Kara Matthews

Kasra Hosseini

Mathew Domeier

SCIENTIFIC REPORTS

OPEN

On the consistency of seismically imaged lower mantle slabs

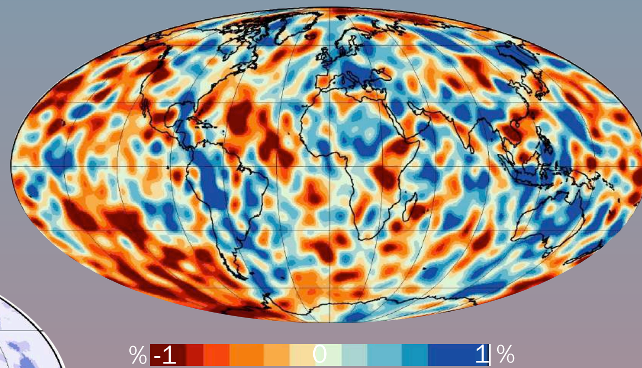
G. E. Shephard[1], K. J. Matthews[2], K. Hosseini[2] & M. Domeier[1]

Shephard et al. (2017)

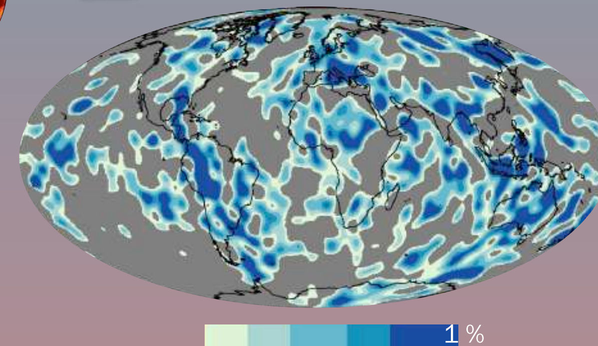
Shephard et al., 2017

Vote maps

1. Base tomography



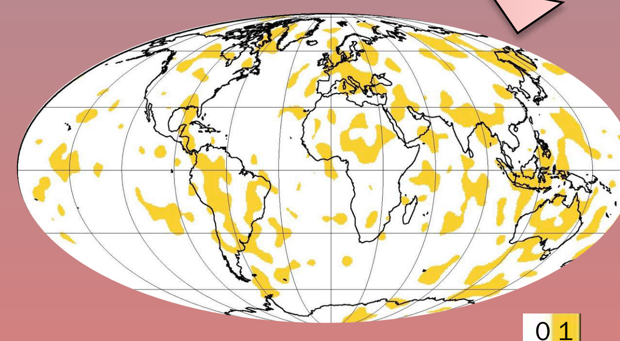
*Retain/**remove**/convert reference model (mean)*



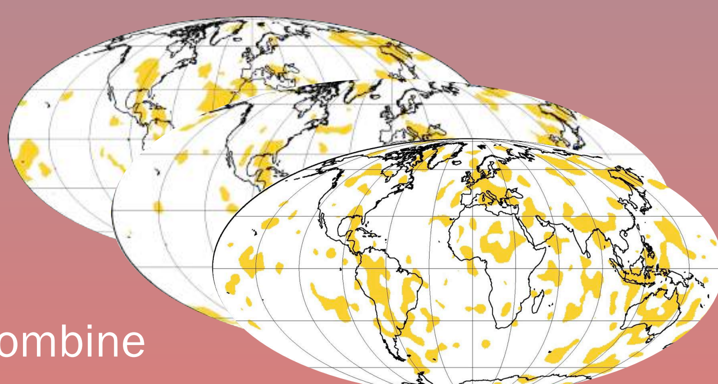
For each depth:

2. Extract positive/negative values

Mean
RMS
St Dev

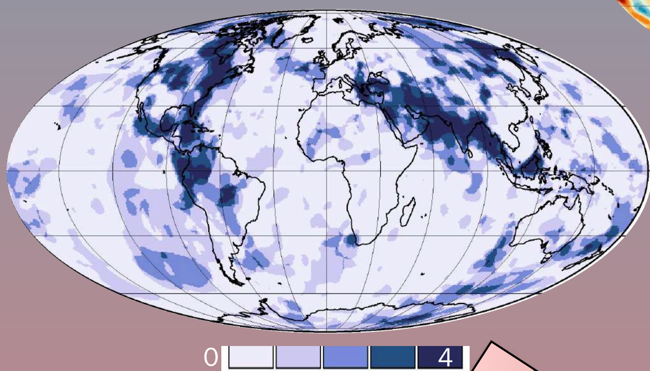


3. Contour



P-waves
S-waves

4. Combine



5. Vote map

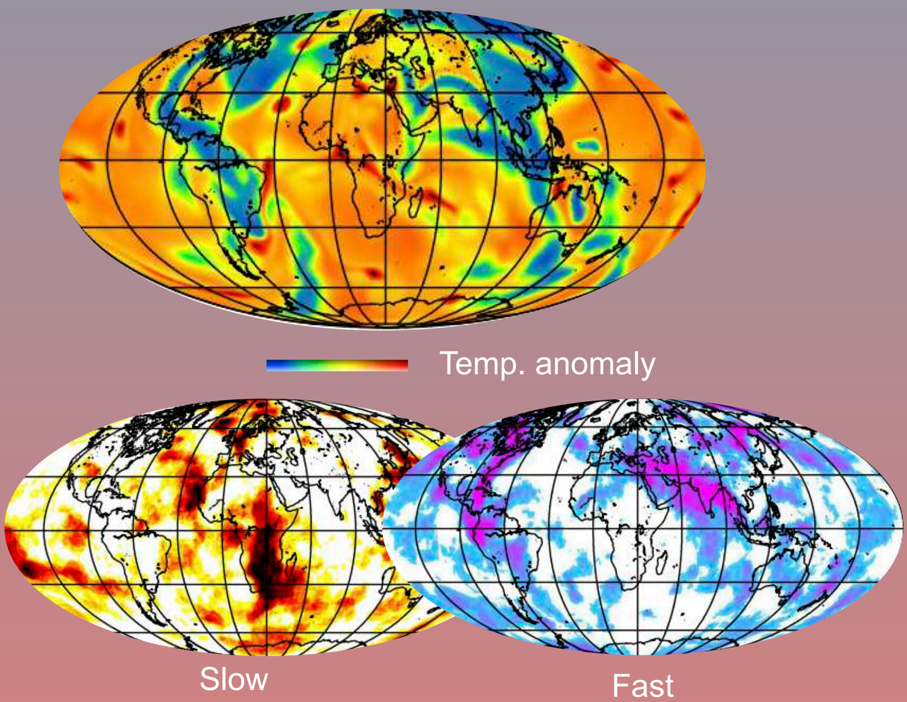
6. Depth analysis

Applications

Geodynamics:

Mantle convection modelling

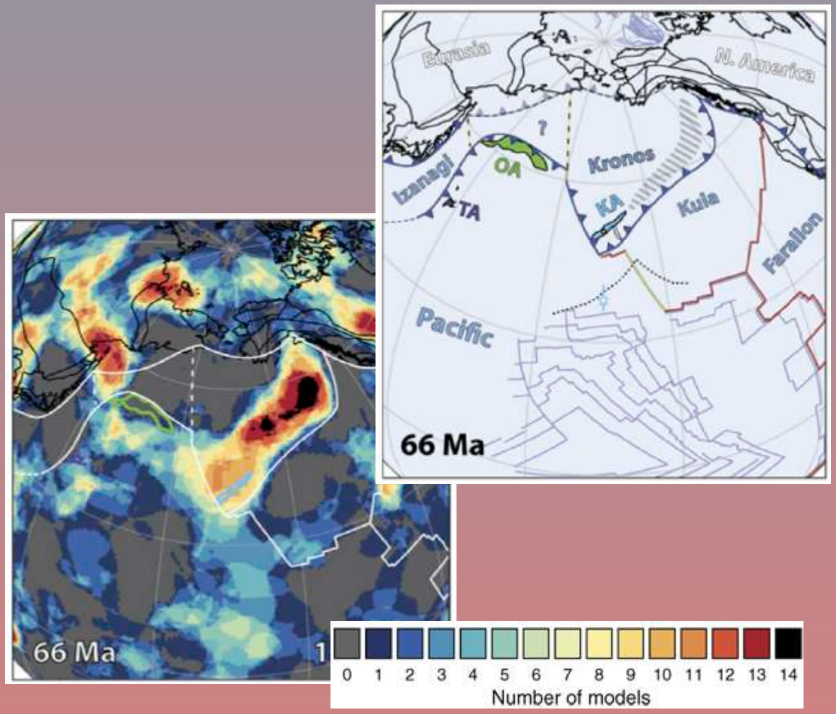
Coltice and Shephard, 2018; JGR



Tectonics:

Origin of Hawaiian-Emperor Bend

Domeier et al., 2017; Science Advances



SubMachine

www.earth.ox.ac.uk/~smachine

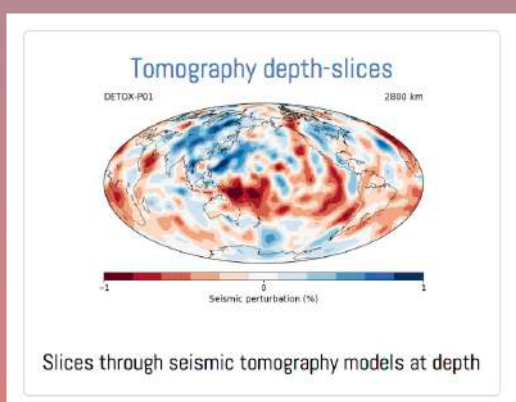
SubMachine

Hosseini et al. (2018)

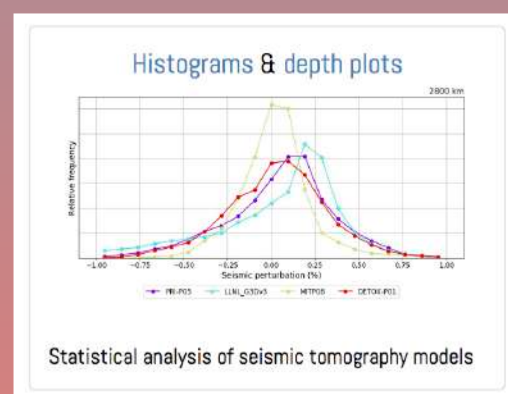
Web-based tools for the interactive visualisation, analysis, and quantitative comparison of global-scale, volumetric (3-D) data sets of the subsurface

- Over 30 tomography models →
- BYO Vote maps

P-wave models	S-wave models
Global tomography models	
GyPSuM-P*	GyPSuM-S*
HMSL-P06*	HMSL-S06*
PRI-P05	PRI-S05
SP12RTS-P	SP12RTS-S
SPani-P*	SPani-S*
Hosseini2016	S20RTS
GAP-P4*	S362ANI+M*
LLNL_G3Dv3*	S40RTS
MITP08*	SAVANI*
MITP_USA_2011MAR*	SAW642ANb*
MITP_USA_2016MAY*	SEMUCB-WM1*
UU-P07*	SEMum*
	SGLOBE-rani*
	TX2011*
	TX2015*
	SEISGLOB1*
	SEISGLOB2*
Regional/depth restricted models	
Sigloch_NAm_2011	3D2016_09Sv*
	SL2013sv*
	Zaroli2016



Slices through seismic tomography models at depth



Statistical analysis of seismic tomography models

Vote maps

	P-wave models	S-wave models	
Hosseini et al., 2016/ Hosseini and Sigloch 2015	DETOX-P01	SEMUCB-WM1	French et al., 2014
Obayashi et al., 2013/ Fukao et al., 2013	GAP-P4	SAVANI	Auer et al., 2014
Houser et al., 2008	HMSL-P06	HMSL-S06	Houser et al., 2008
Burdick et al., 2012	MITP_2011	S40RTS	Ritsema et al. 2011

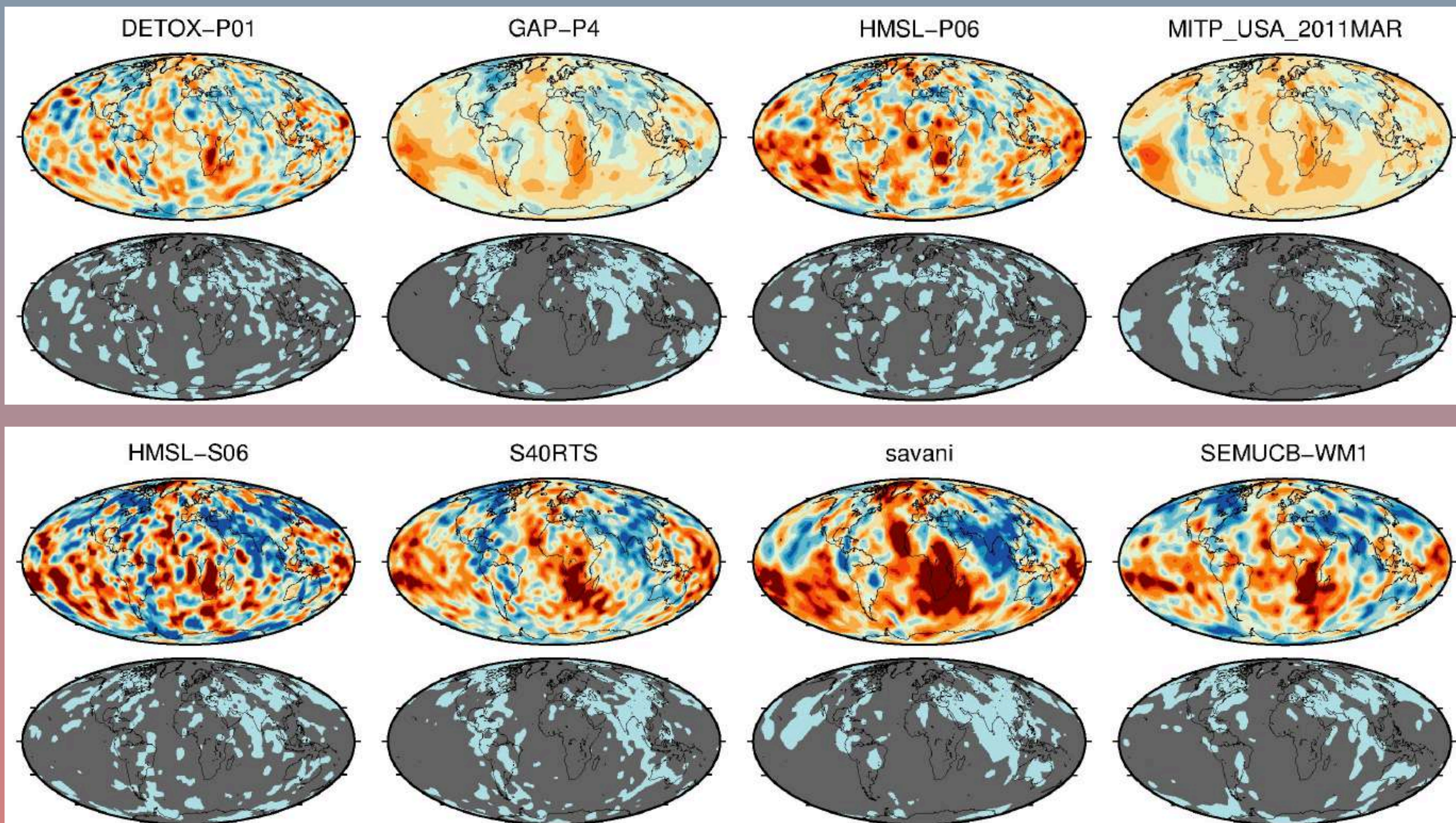
body ± surface ± normal modes ± waveform inversions

0.5° grid spacing
50 km increments
Processed with GMT v5.3.1

Vote maps

Fast anomalies

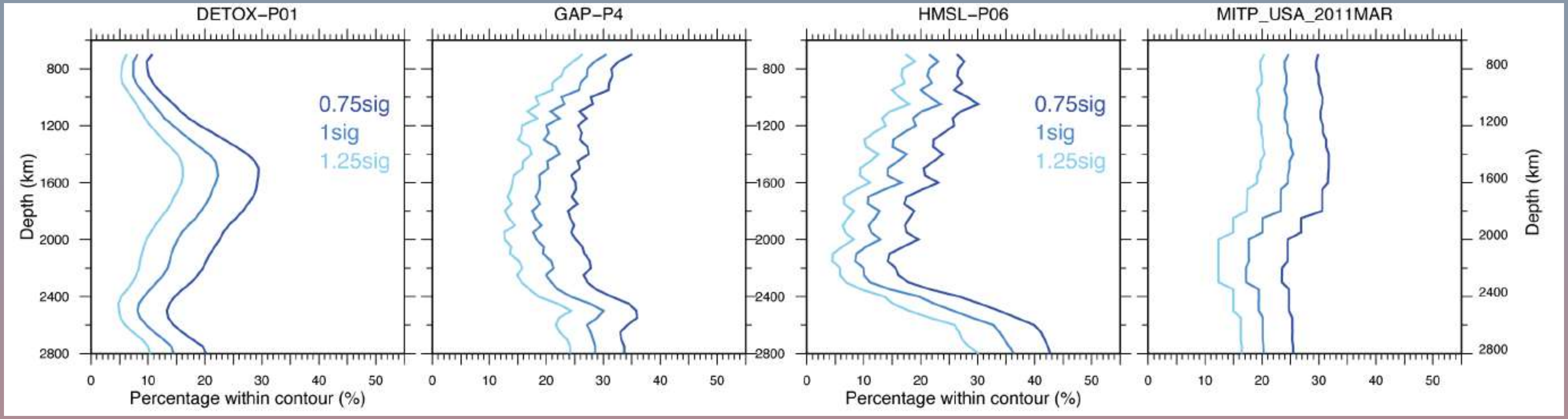
contour >+1σ 1800 km



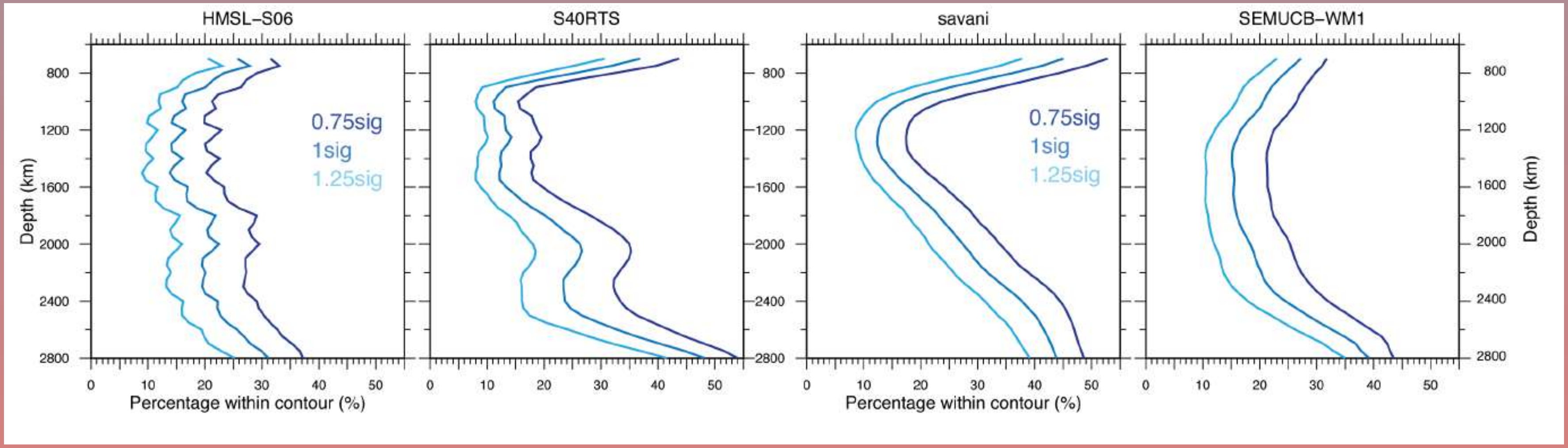
Vote maps – contour

Fast anomalies

P-waves



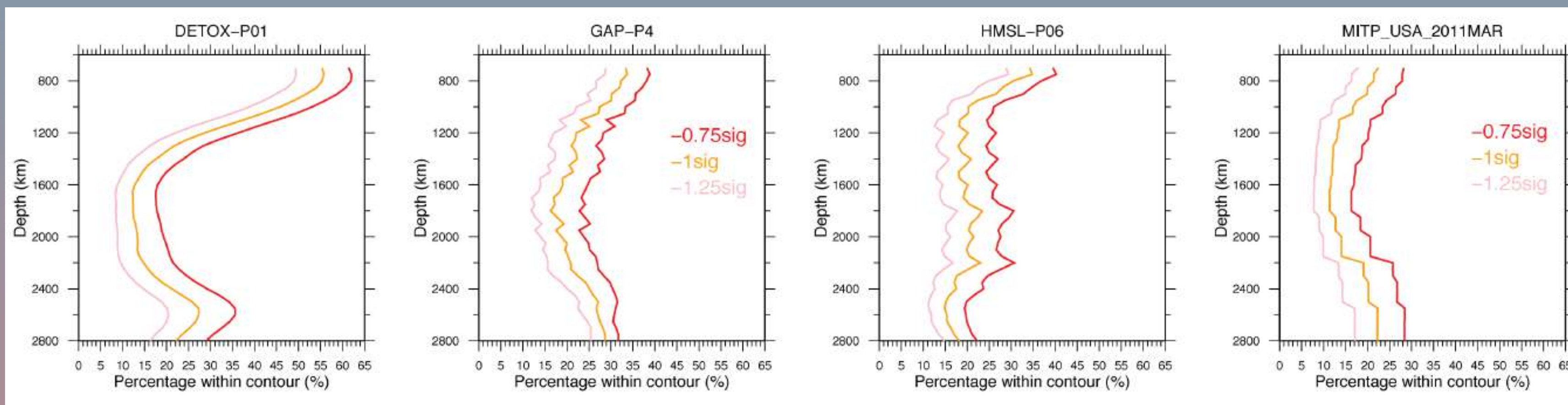
S-waves



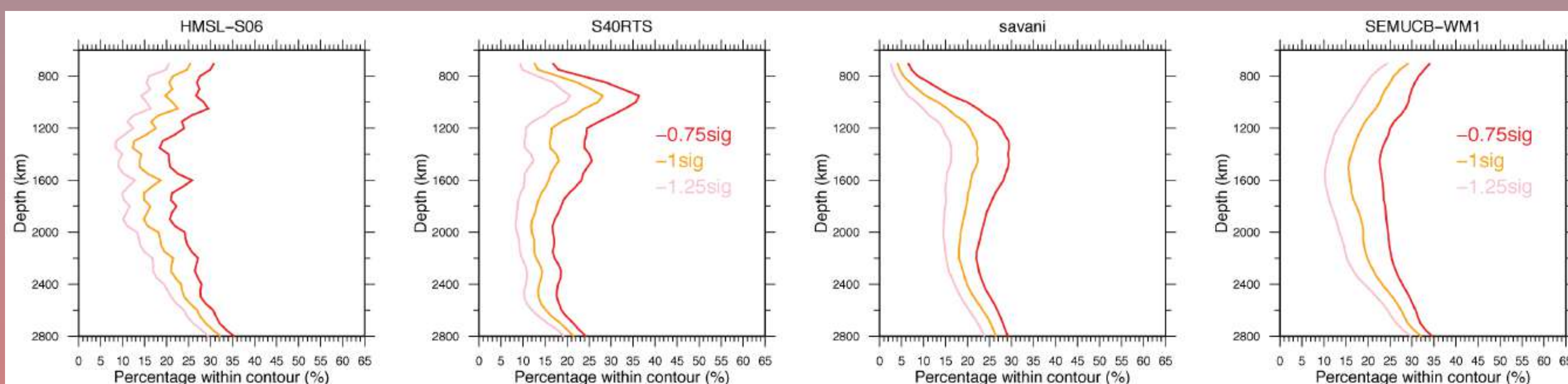
Vote maps – contour

Slow anomalies

P-waves



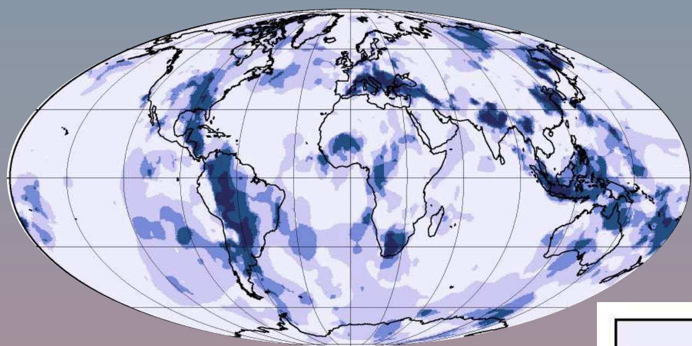
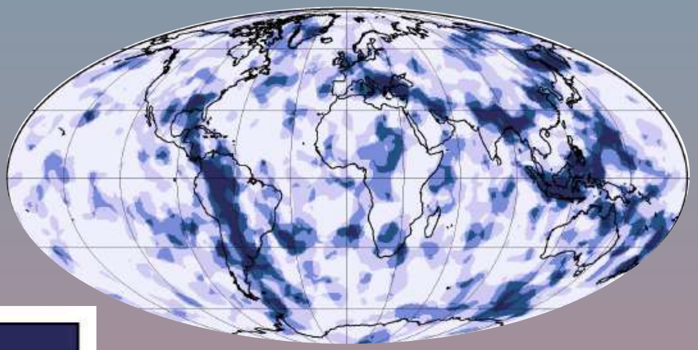
S-waves

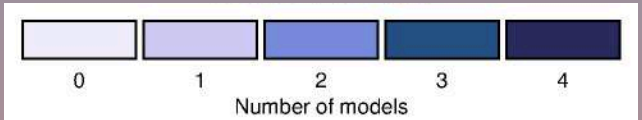


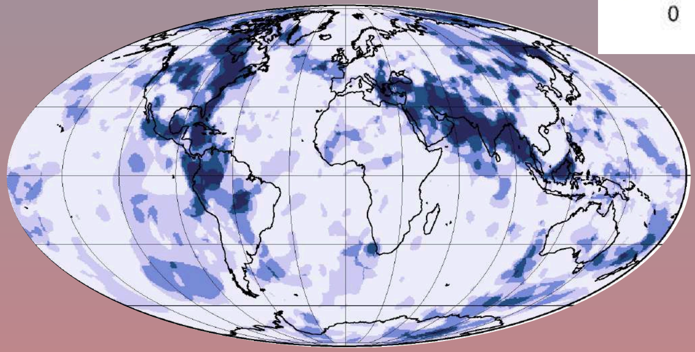
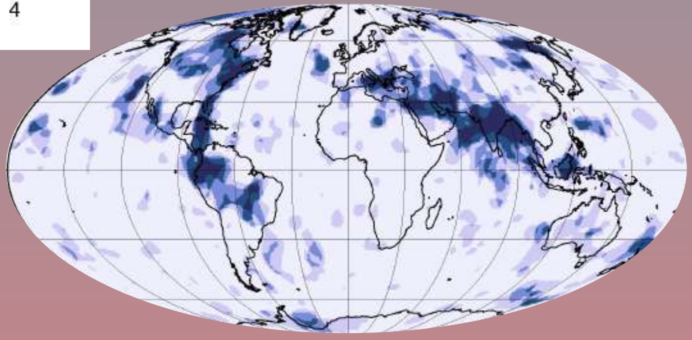
>+1σ

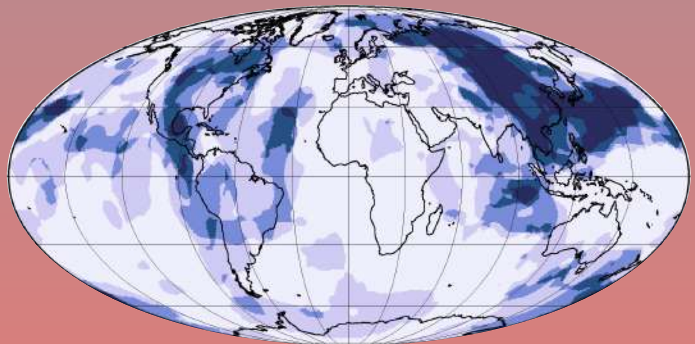
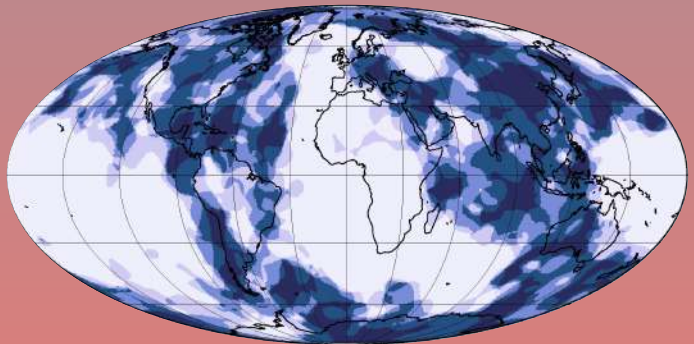
Fast anomalies

V_P | V_S


800 km


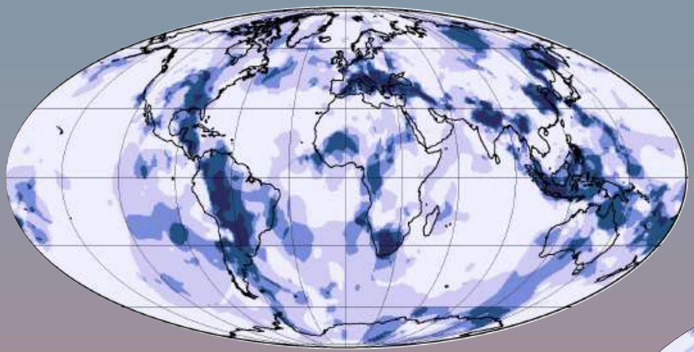



1400 km


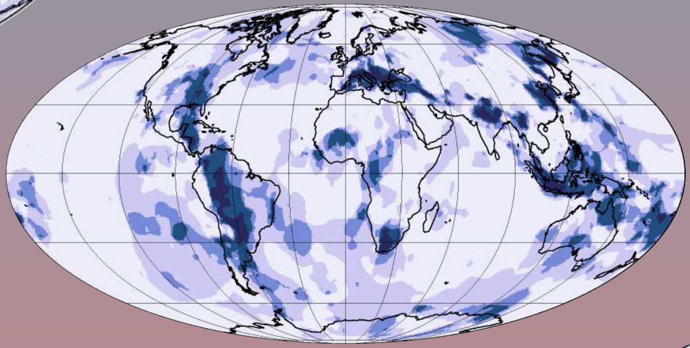

2800 km


Influence of sigma

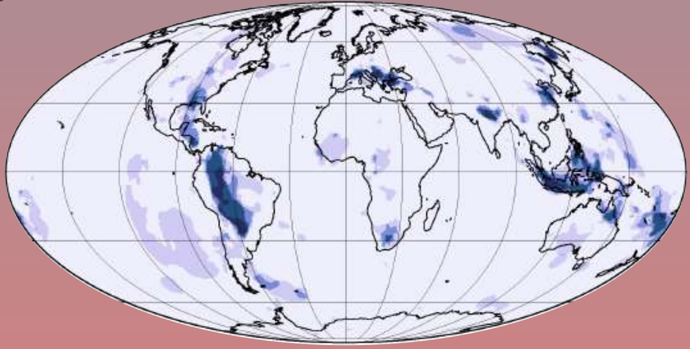
>+0.75σ

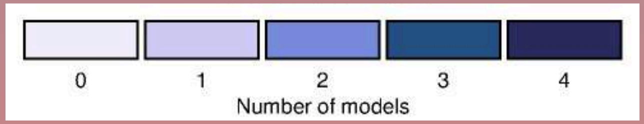


>+1σ



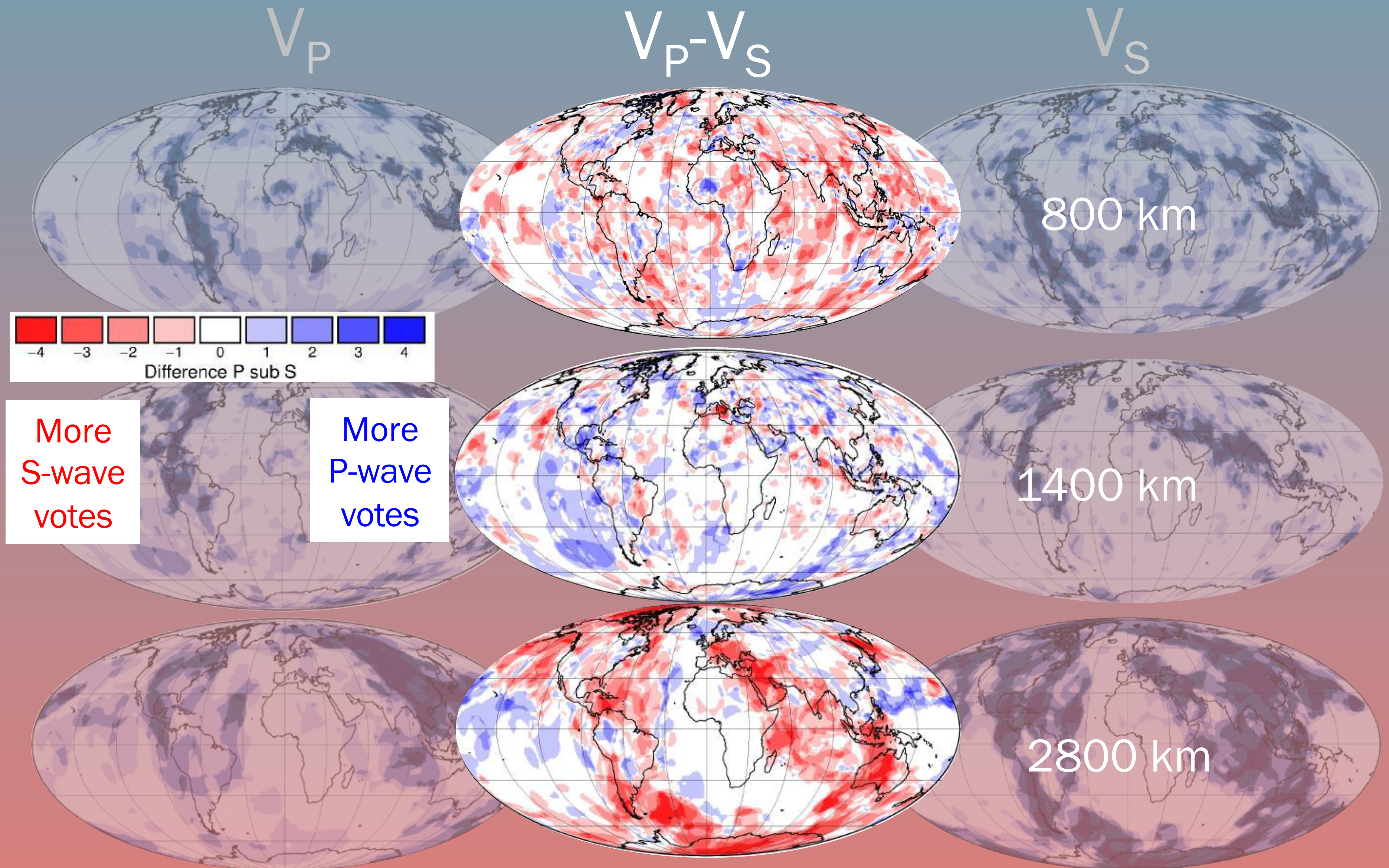
>+2σ





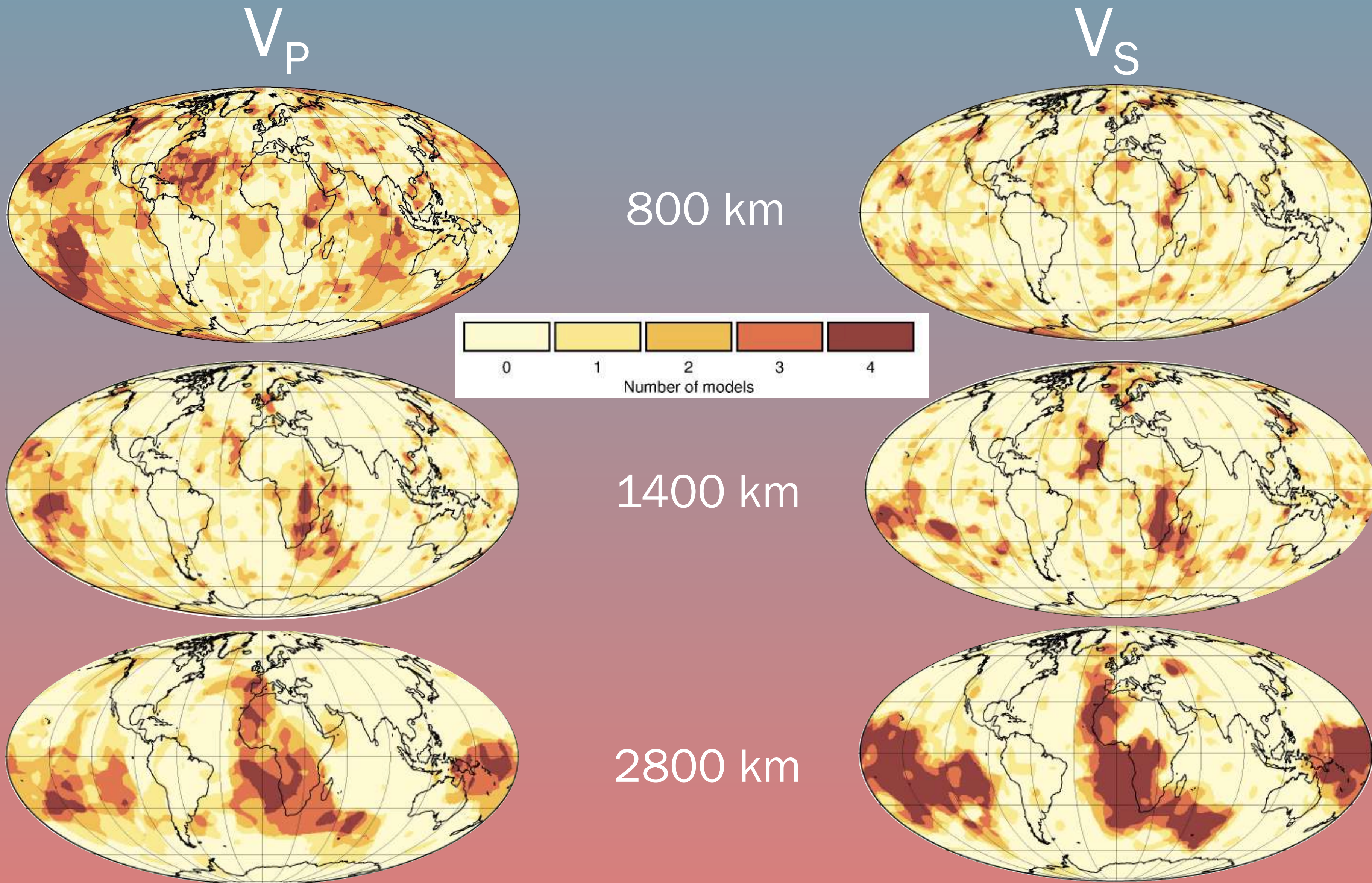
Fast anomalies

>+1σ



Slow anomalies

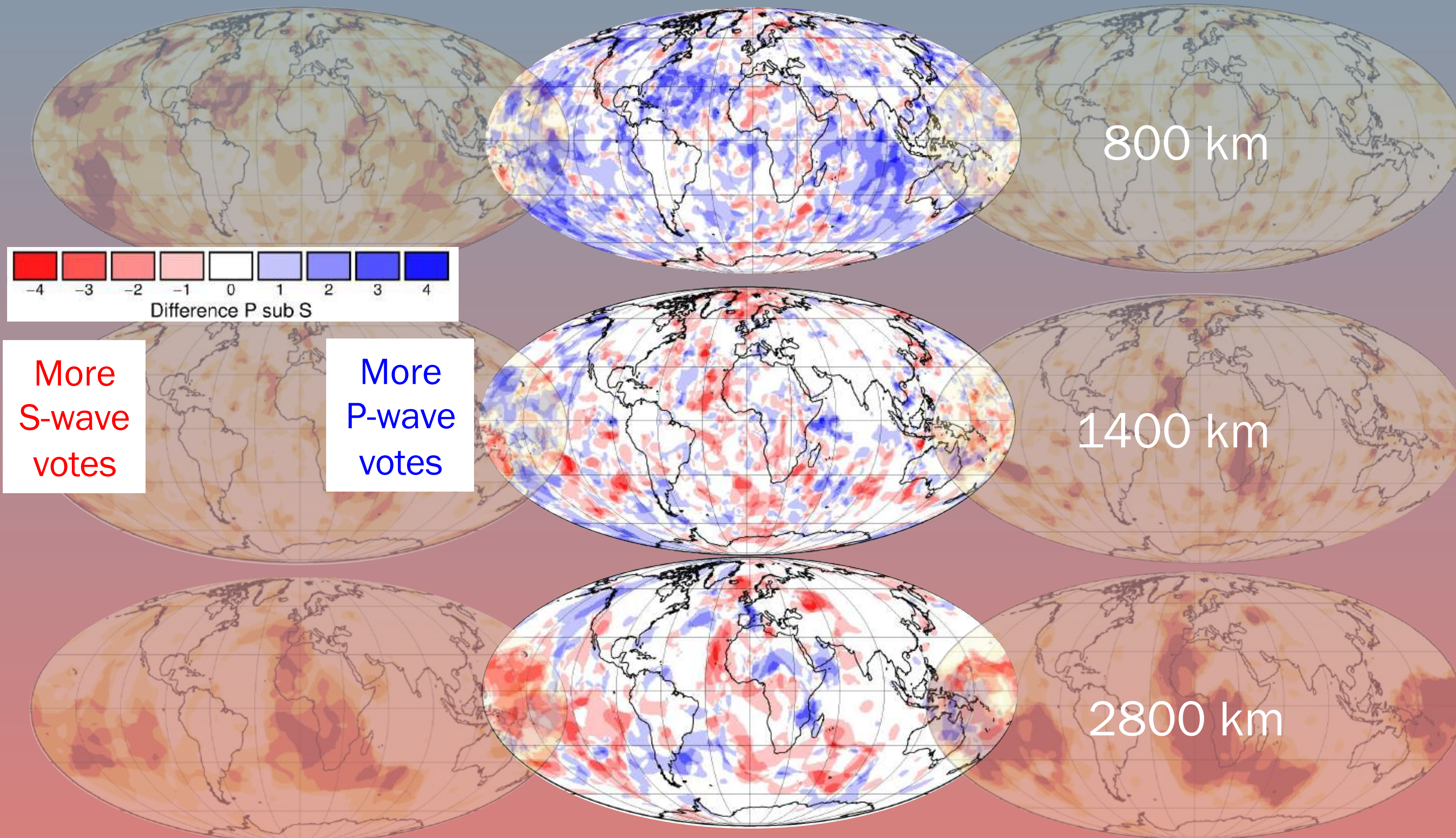
<-1σ



Slow anomalies

<-1σ

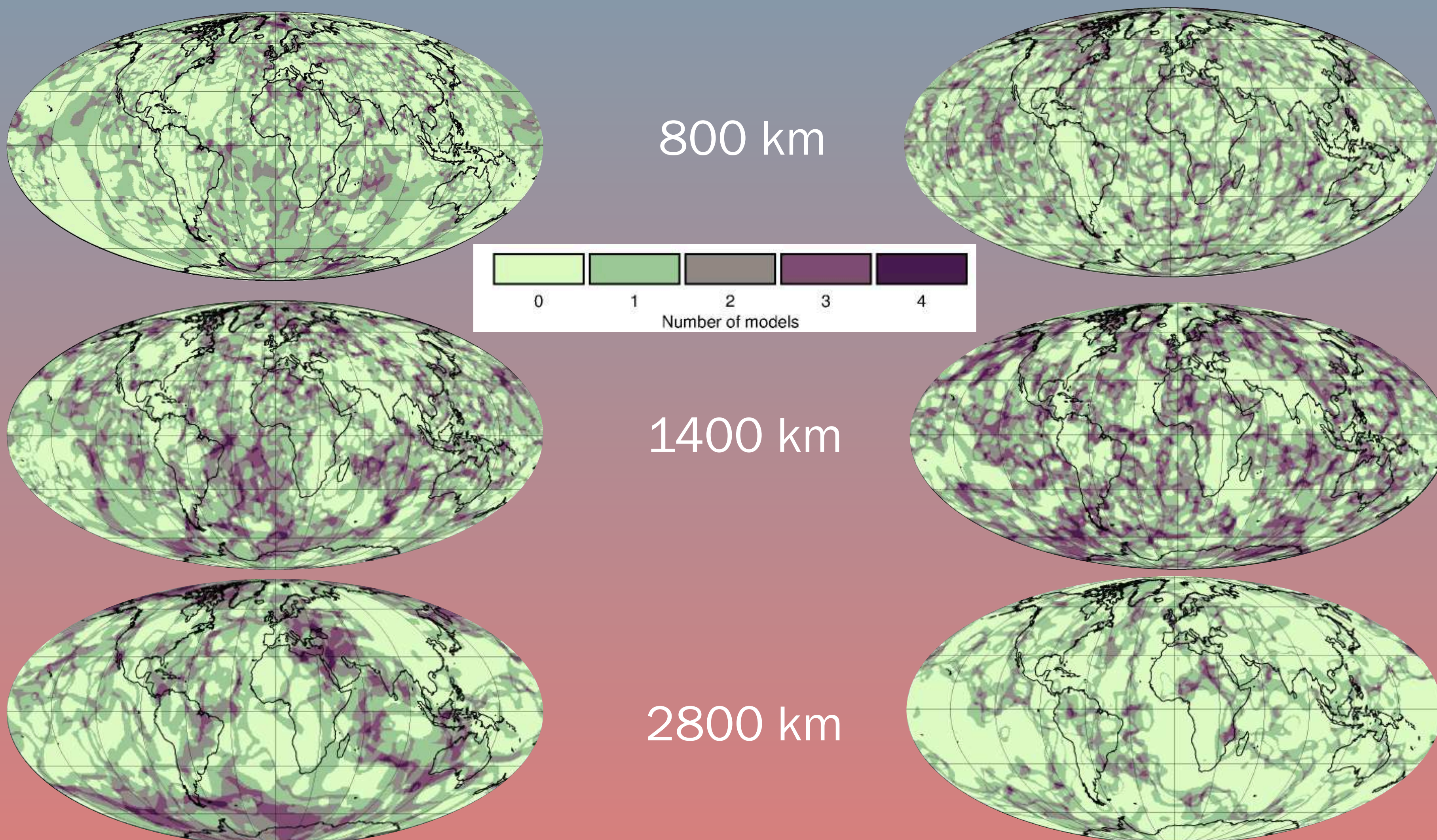
V_P | V_P-V_S | V_S



Ambient “anomalies”

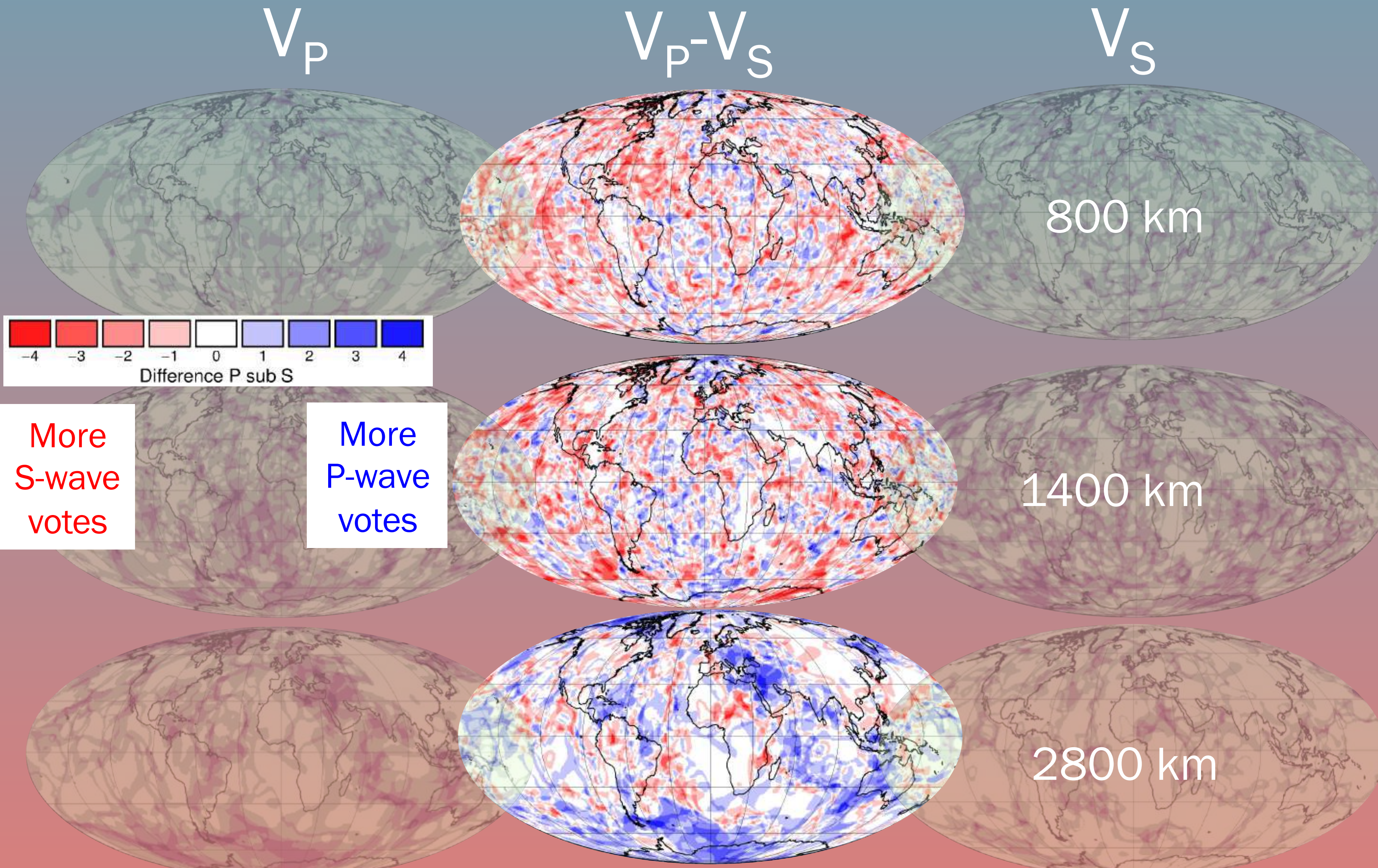
±0.5σ

V_P V_S

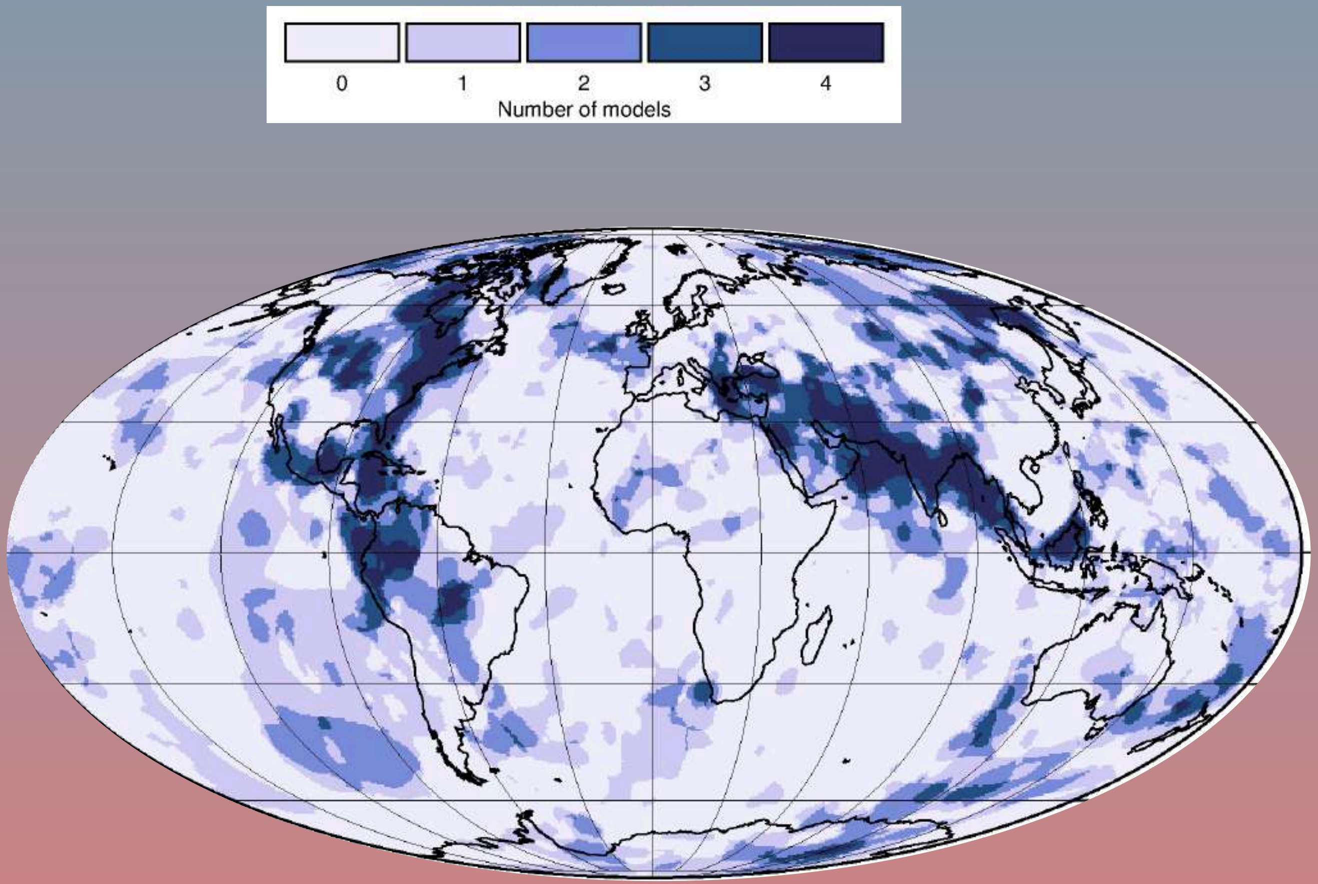


Ambient "anomalies"

±0.5σ

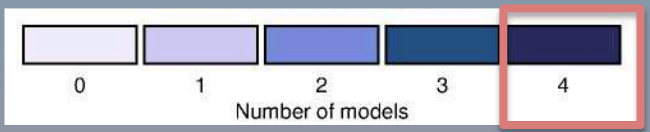


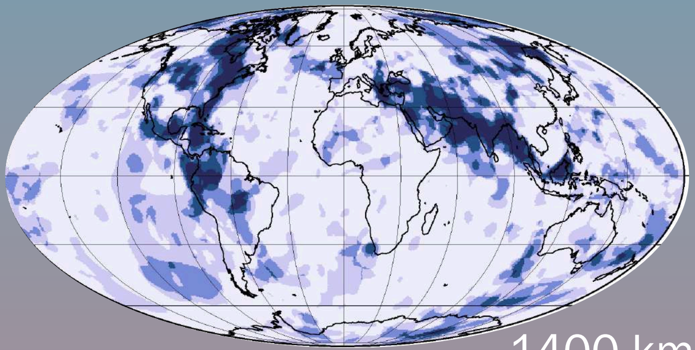
Surface area calculations



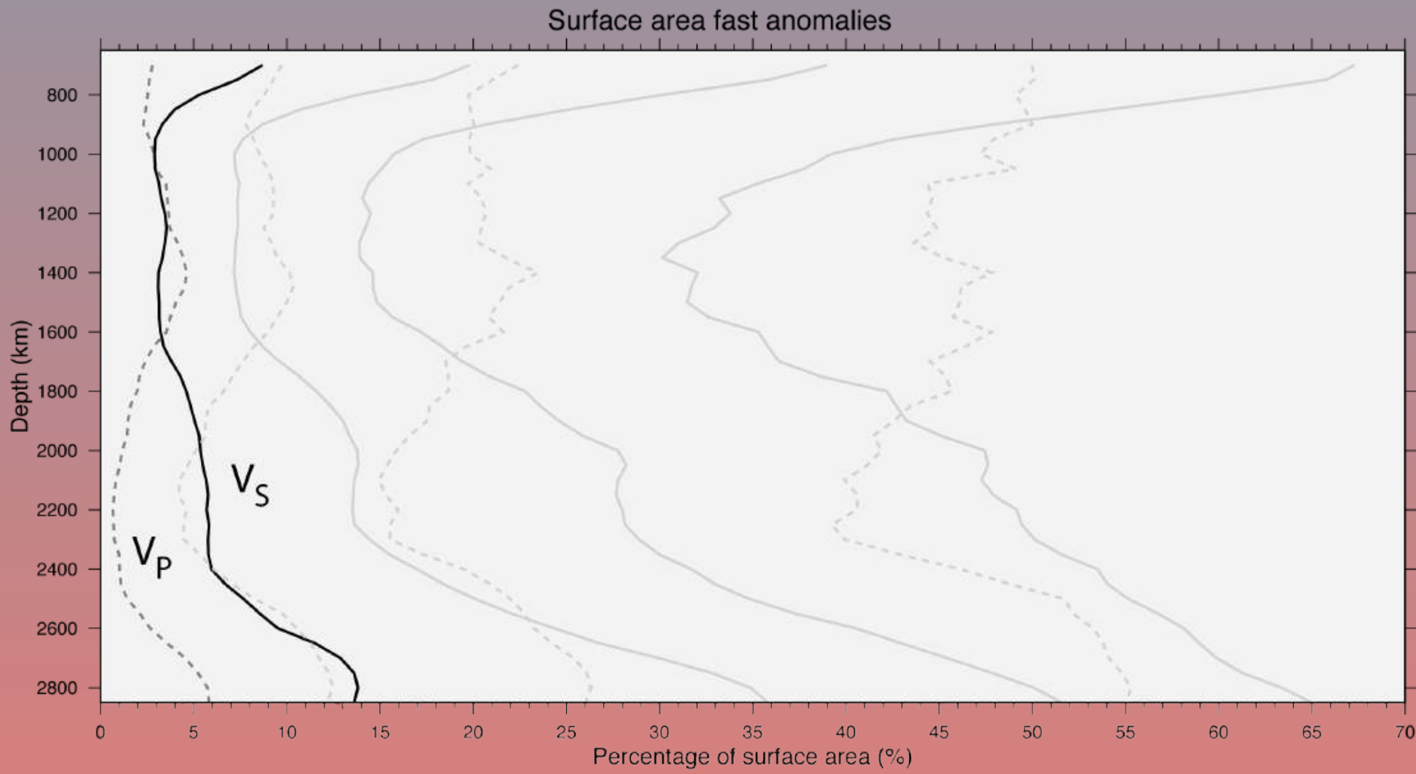
1400 km

Surface area calculations

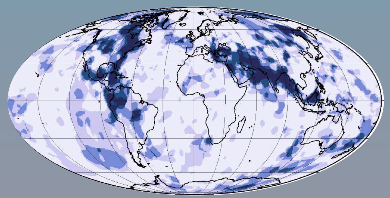


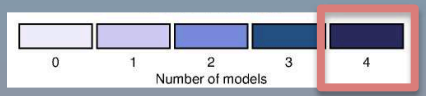


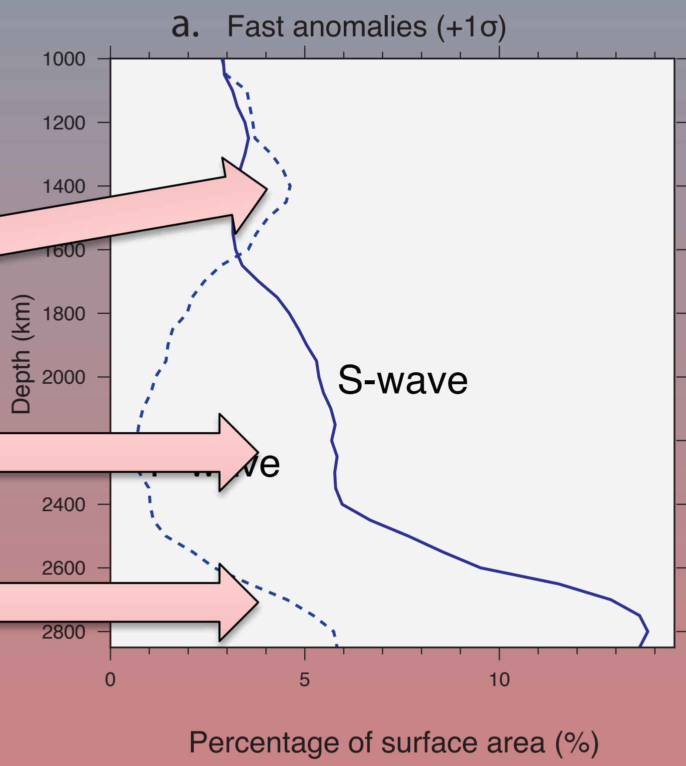
1400 km



Change in coverage







Onset of decorrelation below 1400 km

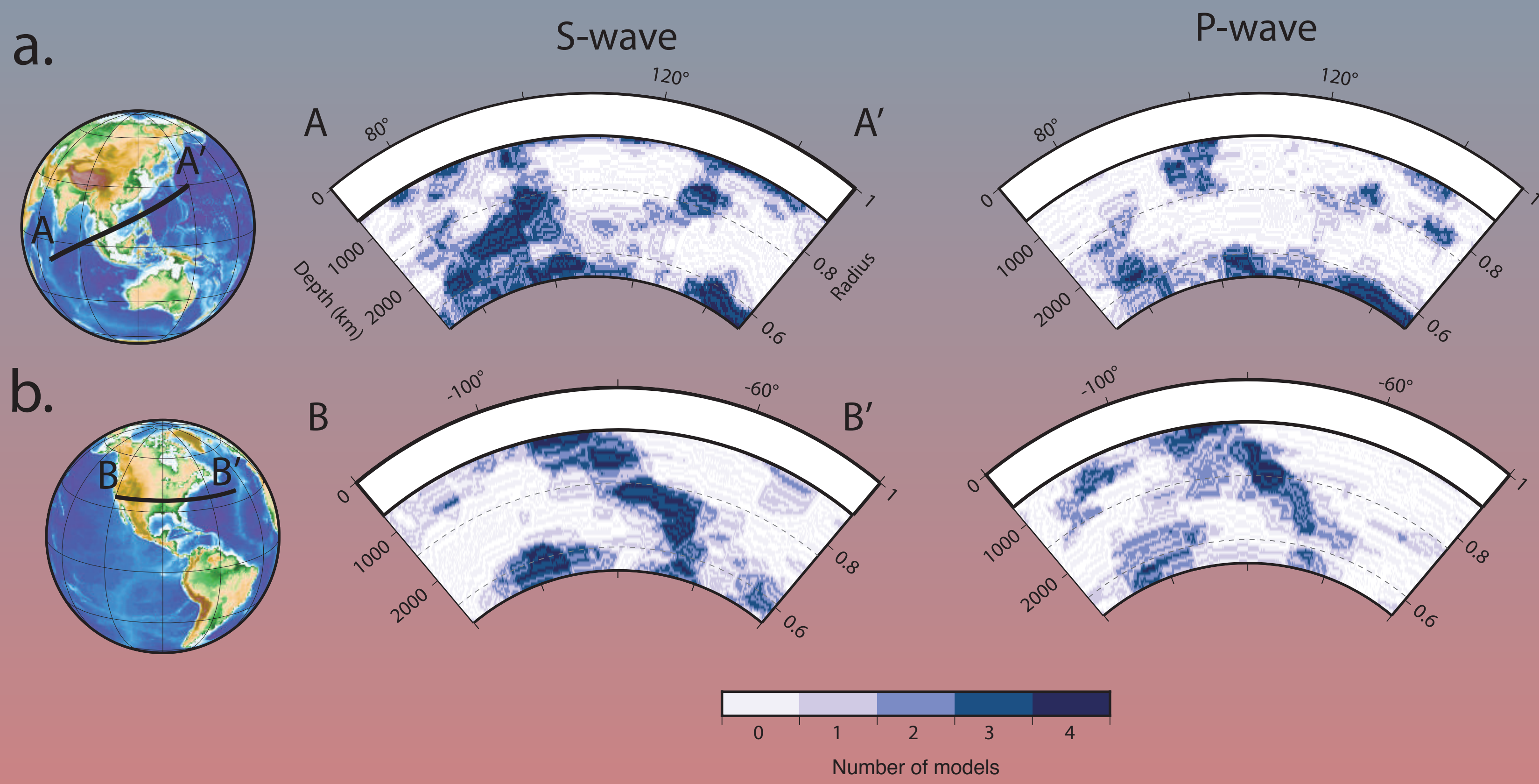
Matching again below 2200 km

Slab graveyard and LLSVP effect

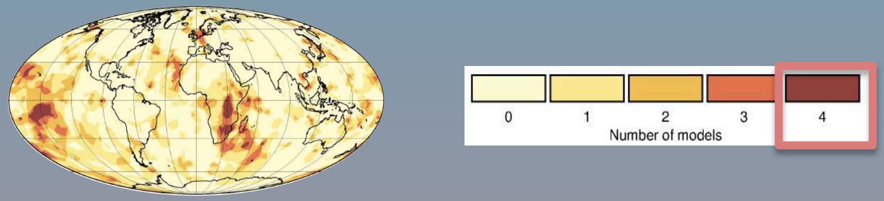
<u>Fast anomalies</u>

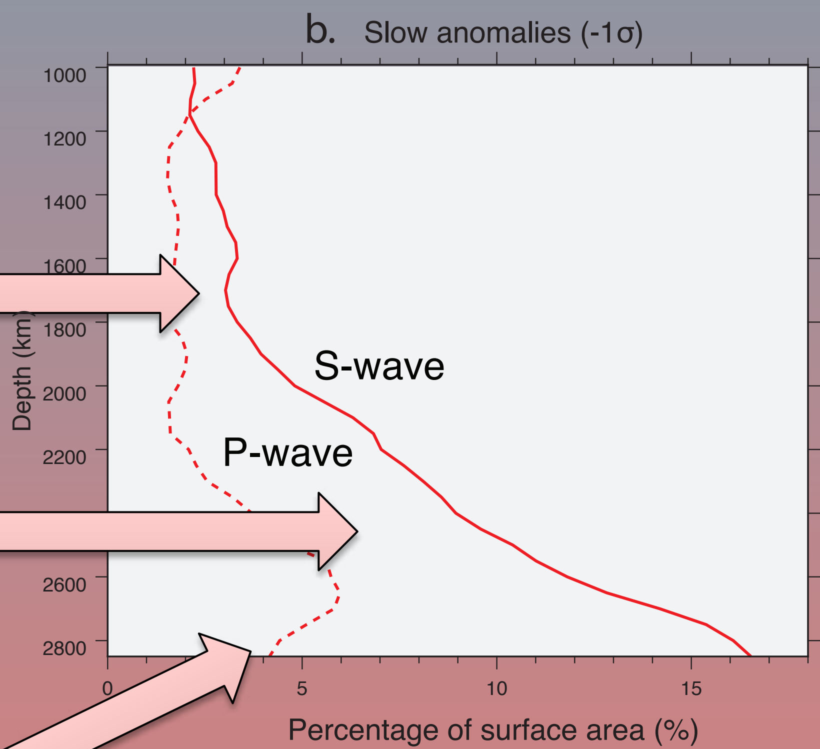
- Clear mid-mantle decorrelation

Fast anomalies



Change in coverage





Onset of decorrelation ~1700 km

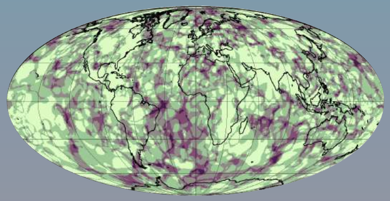
Slab graveyard and LLSVP effect

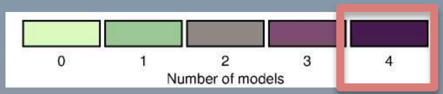
Post-perovskite(?)

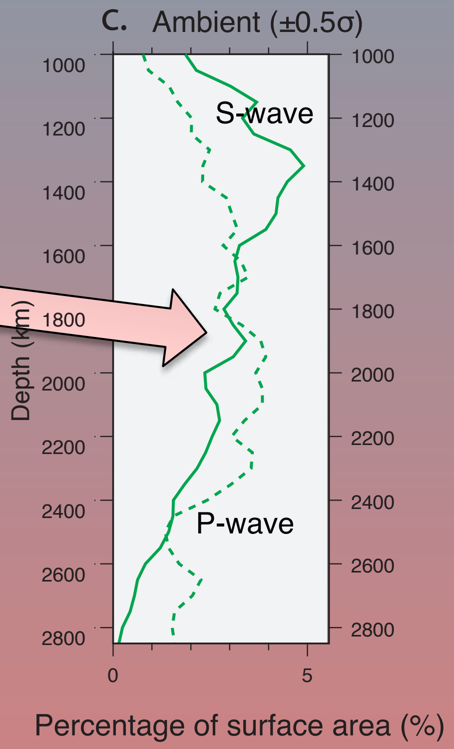
<u>Slow anomalies</u>

- Deeper mid-mantle decorrelation
- LLSVP effects

Change in coverage





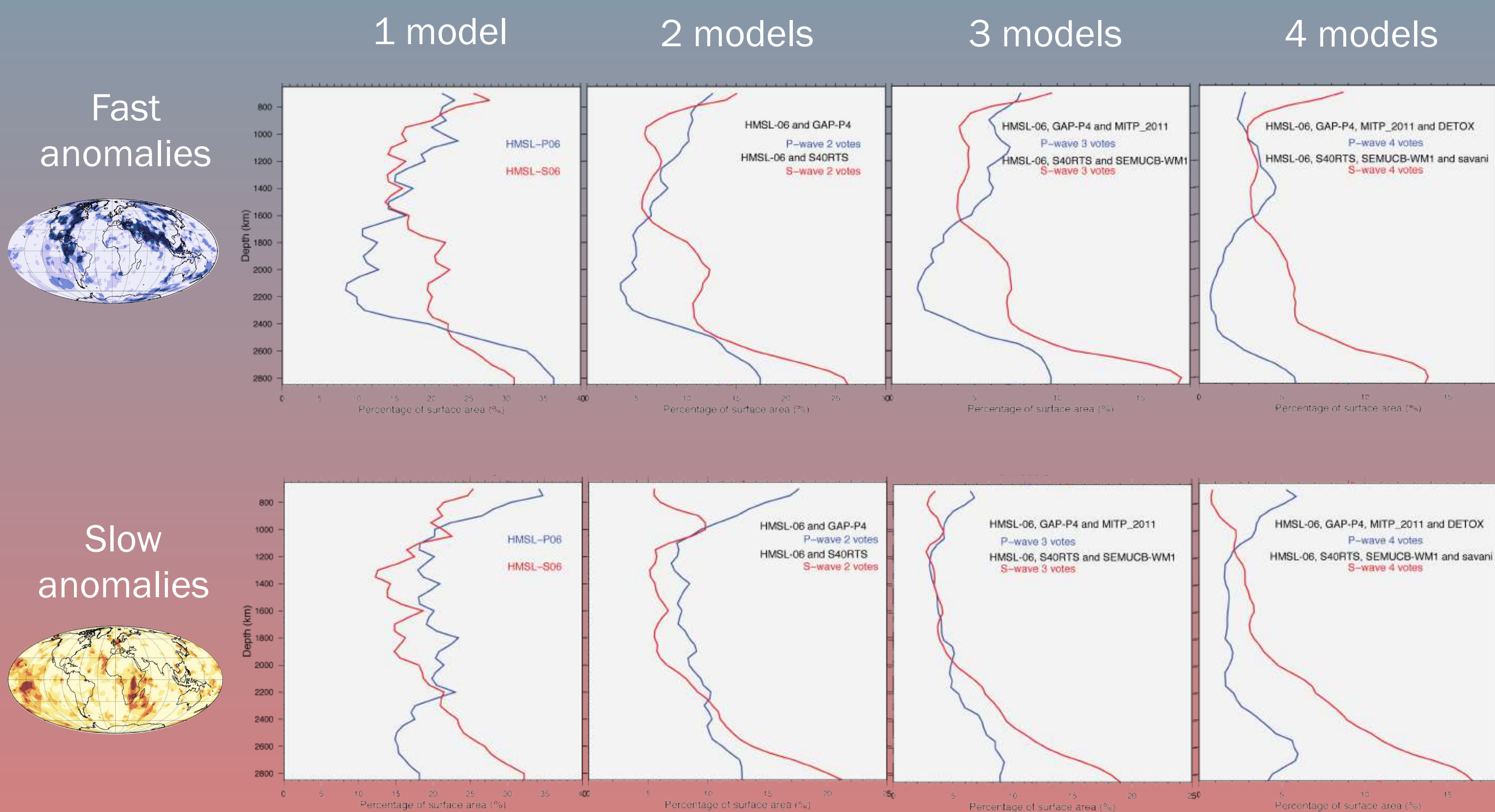


No clear decorrelation

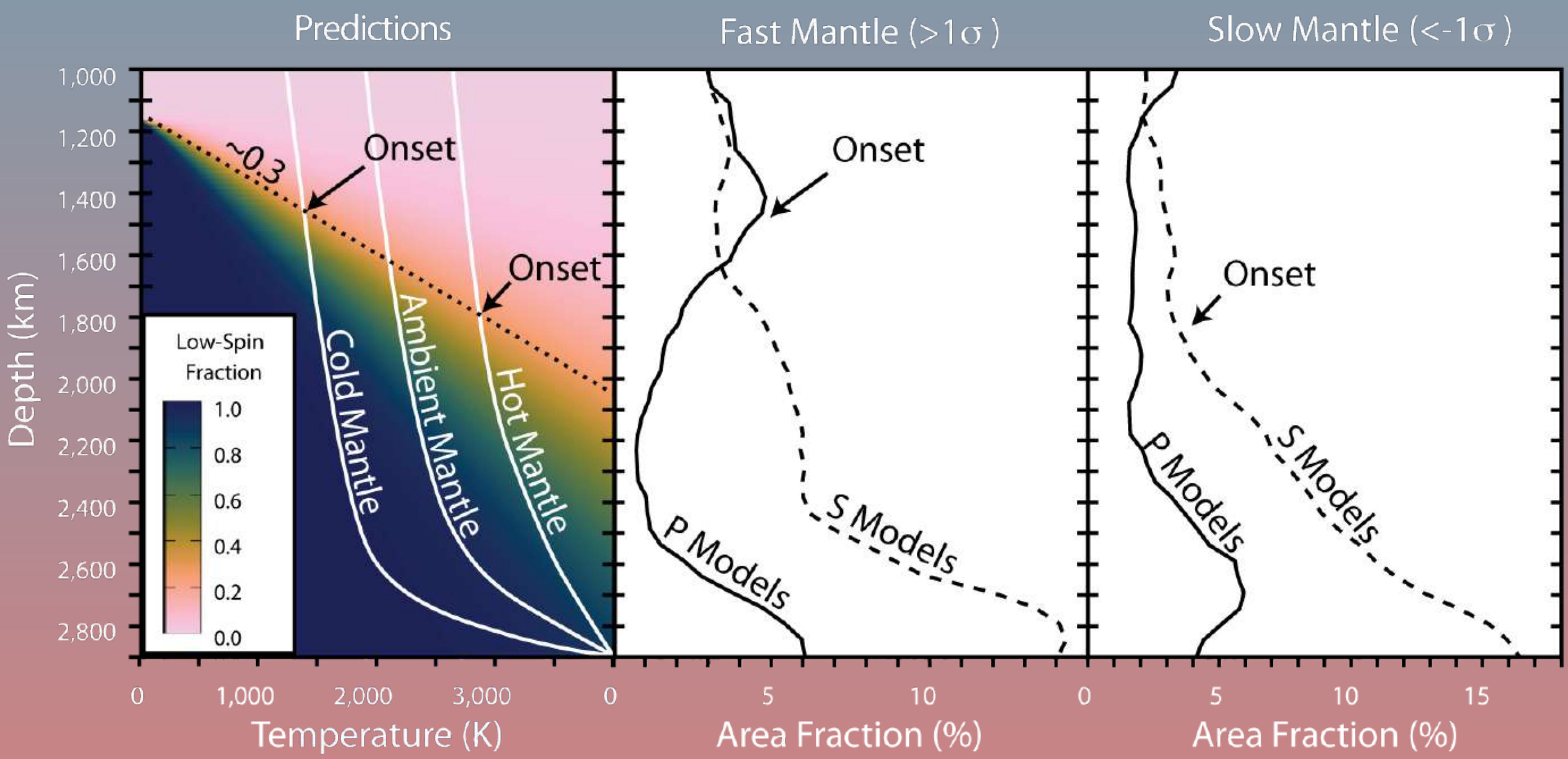
Ambient domain

- No clear signal

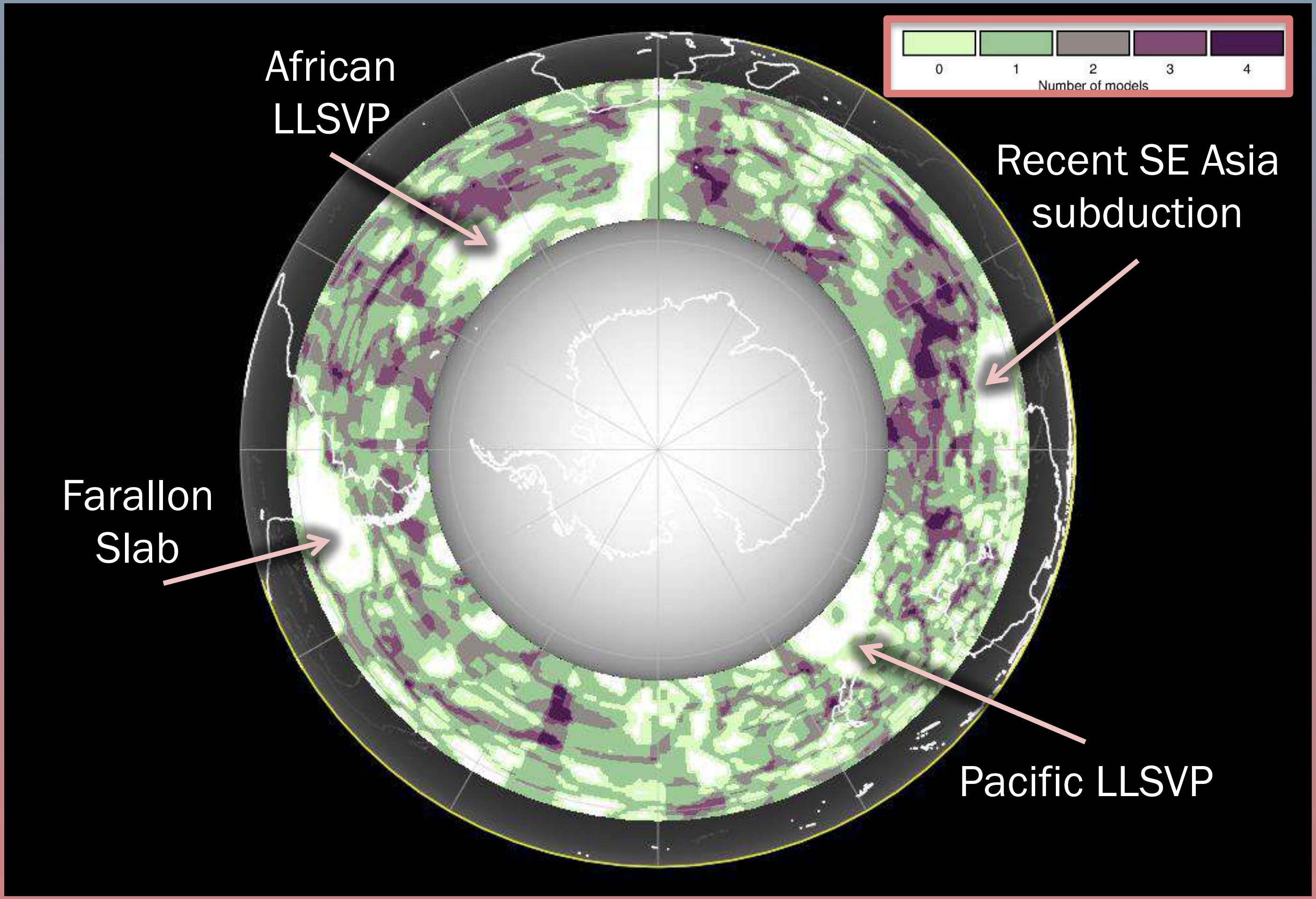
Different tomography combos



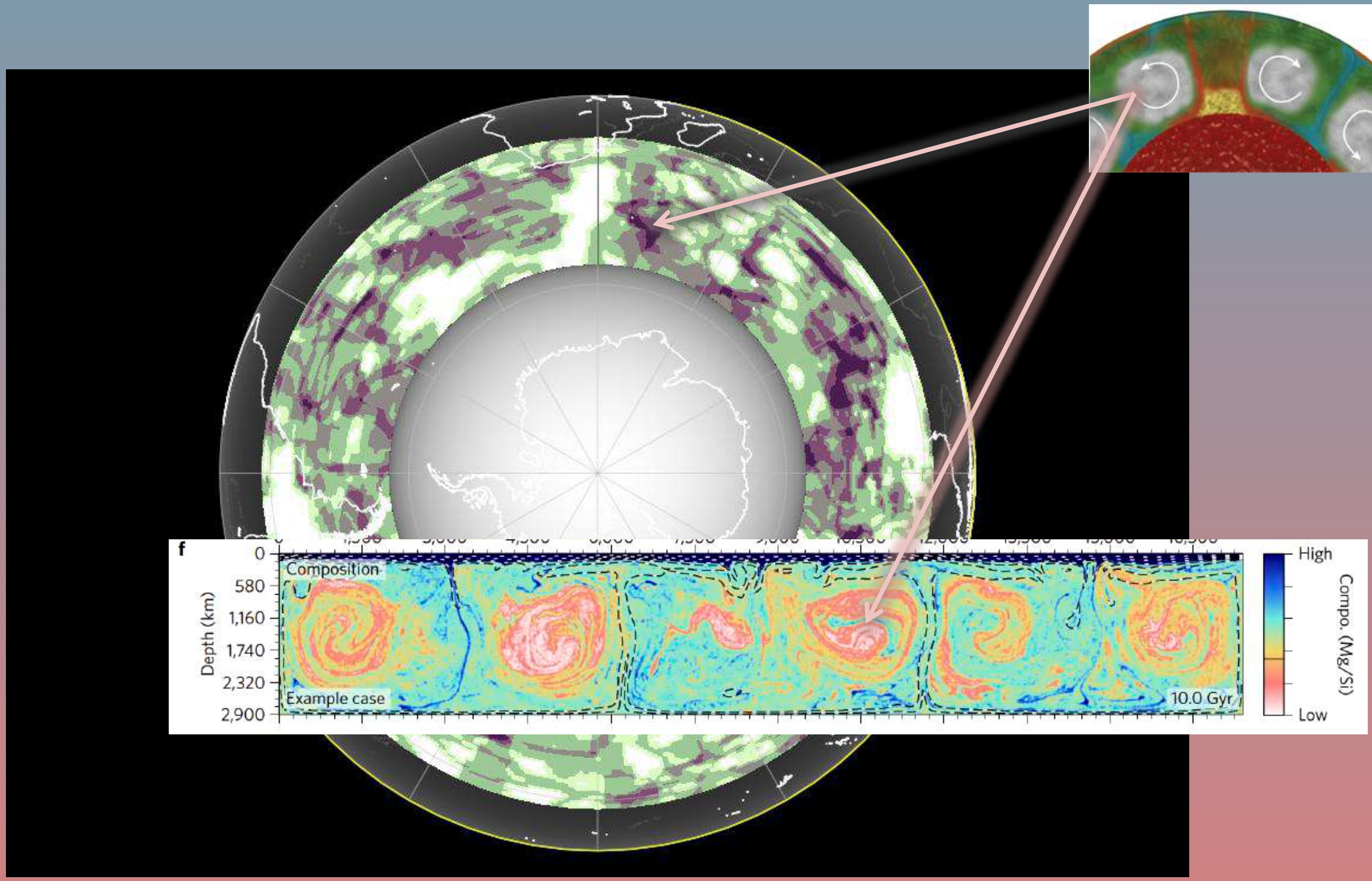
Change in coverage



Ambient mapping

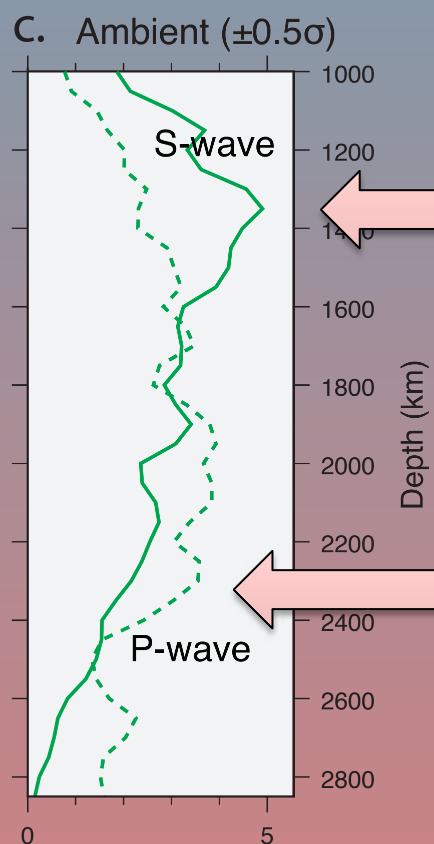


Ambient mapping



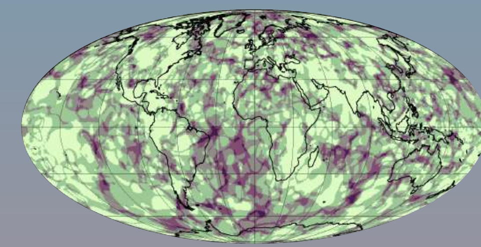
BEAMS (Bm-enriched ambient mantle structures) model; Ballmer et al (2015, 2017)

Ambient mapping



Top of
BEAMS?

Bottom of
BEAMS?



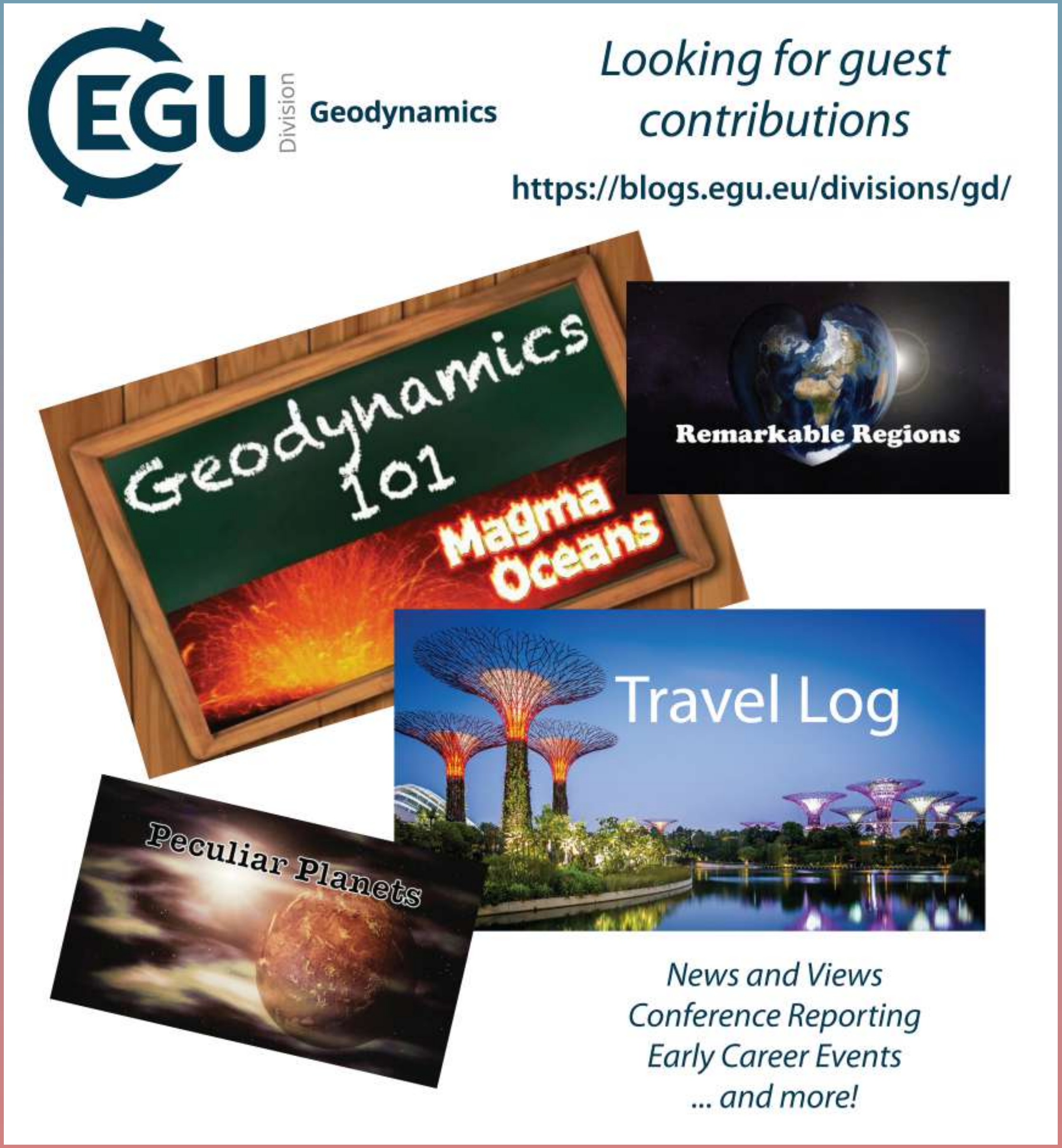
SiO_2 rich, not readily mixed,
rheologically strong,
neutrally buoyant

EGU GD Blog

Weekly blog posts (Wednesdays)

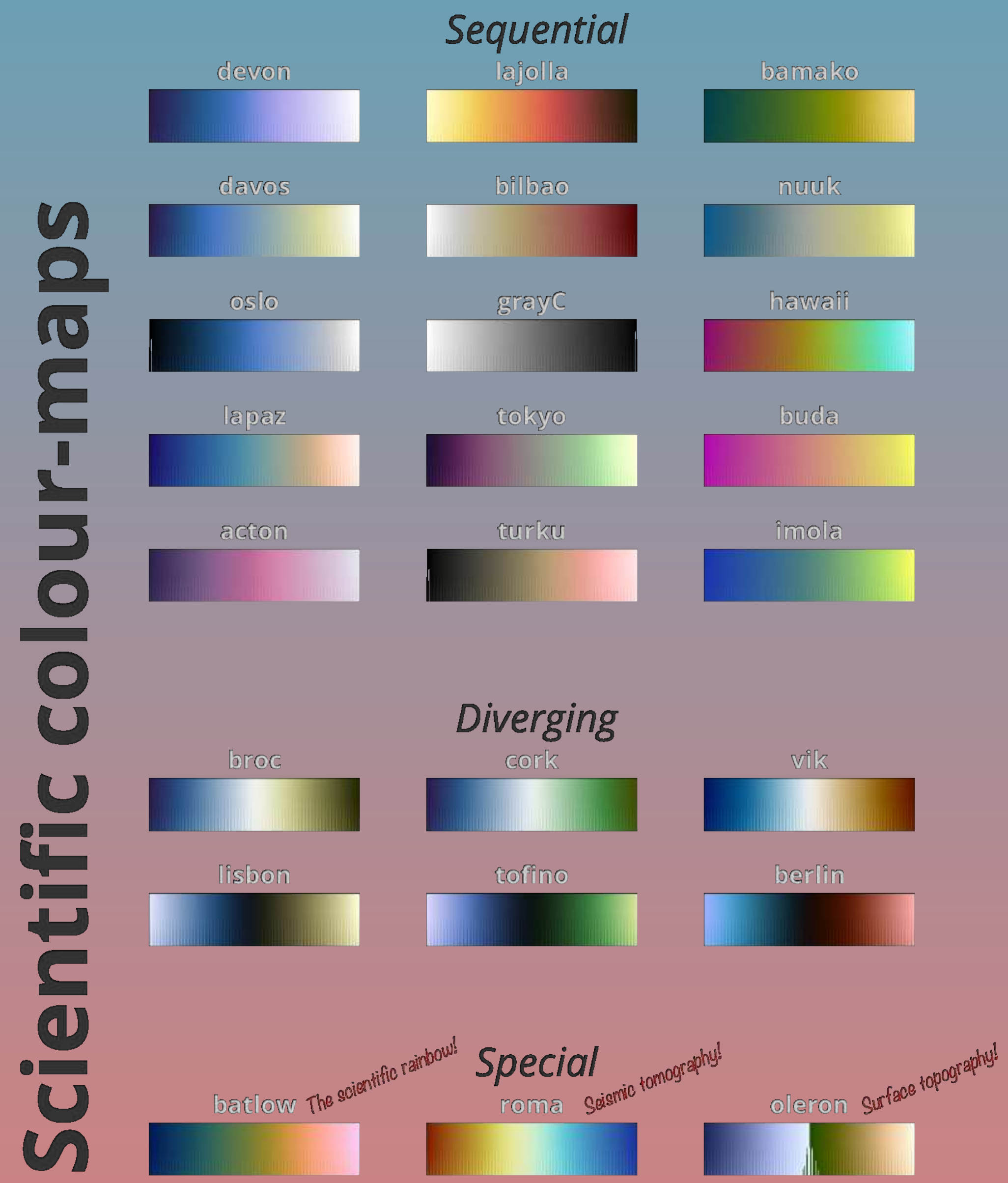
Looking for guest authors!

Speak to:
Diogo Lorenço
Antoine Rozel
Anna Gülcher
Anne Glerum
Tobias Meier



Scientific Colour Maps

www.fabiocrameri.ch/colourmaps.php



Crameri (2018)

www.fabiocrameri.ch

Conclusions

- Changes in volume necessitate changes in bulk modulus
- Spin transition can be detected by evaluating multiple Vp and Vs tomography models
  - Below ~1400 km in fast/cold regions
  - Below ~1700 km in slow/warm regions
- Ambient mantle likely contains little Fp – SiO_2 enriched
  - Consistent with the BEAMS model