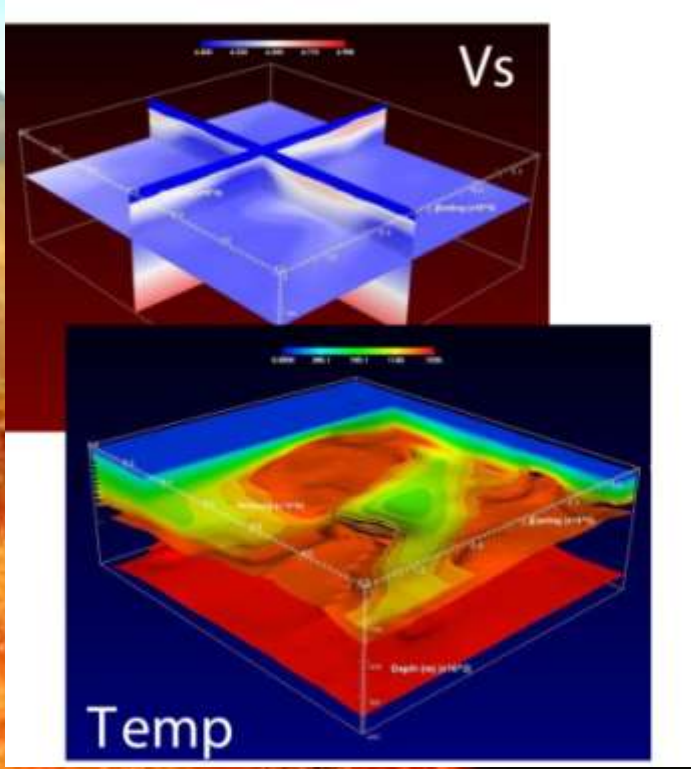
Integrated geophysical and petrological modelling of the uppermost mantle: forward and inversion approaches



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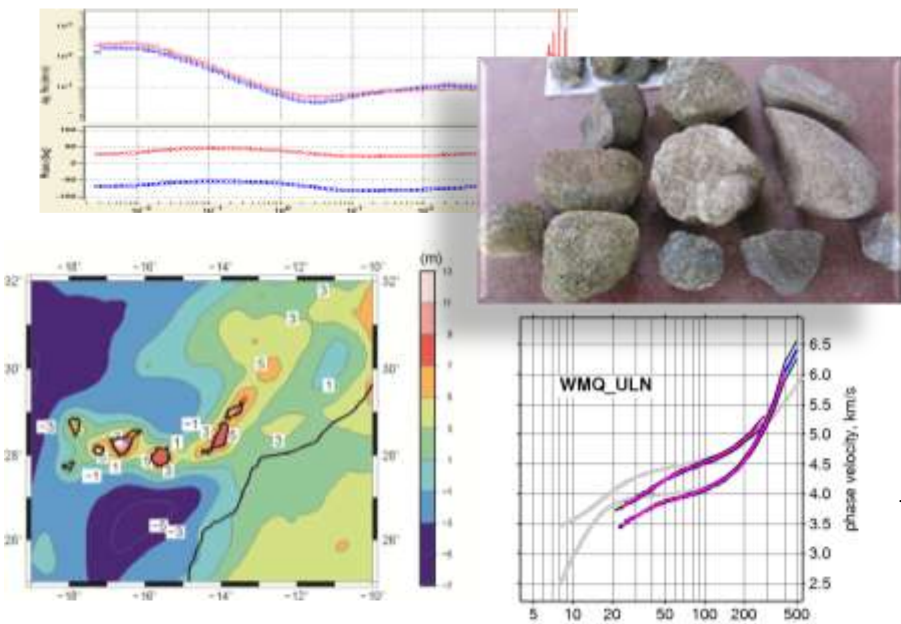
- Integrating (self-consistently) geophysical and petrological data to image the lithosphere/uppermost mantle

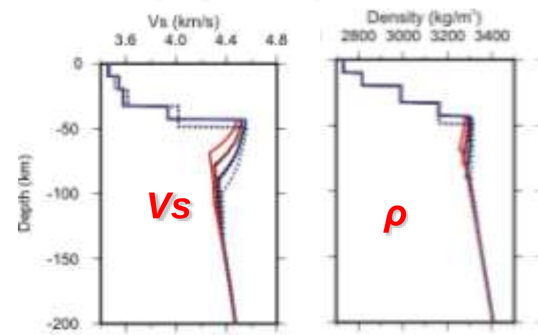
Geophysical & petrological data

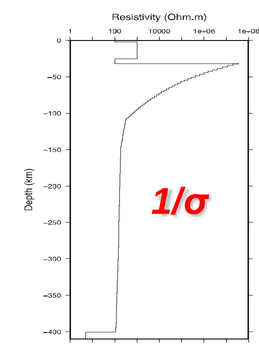


Inversion

Forward modeling

Geophysical parameters





Integrated modelling

Temperature, Pressure, Composition

- Forward approach
- Non-linear probabilistic inversion

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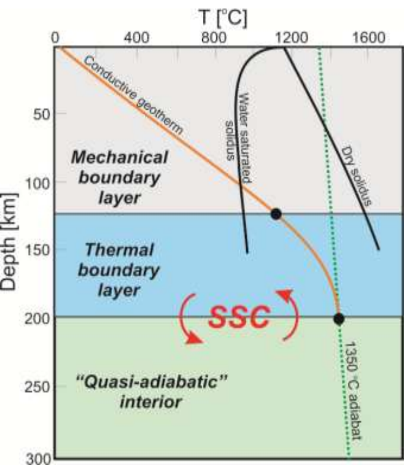
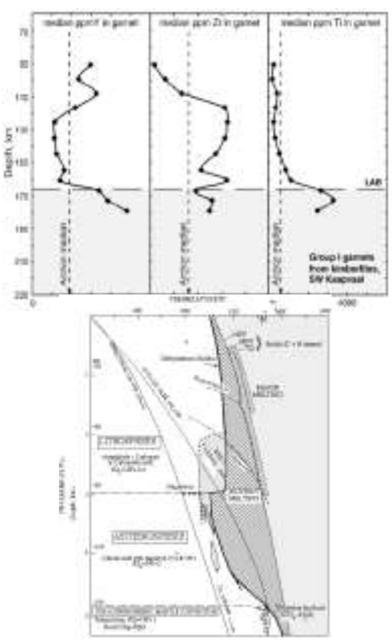
Why integrated modelling...?

A fundamental upper mantle discontinuity for plate tectonics: the lithosphere-asthenosphere boundary (LAB) can be defined as ***thermal, mechanical and chemical boundary***

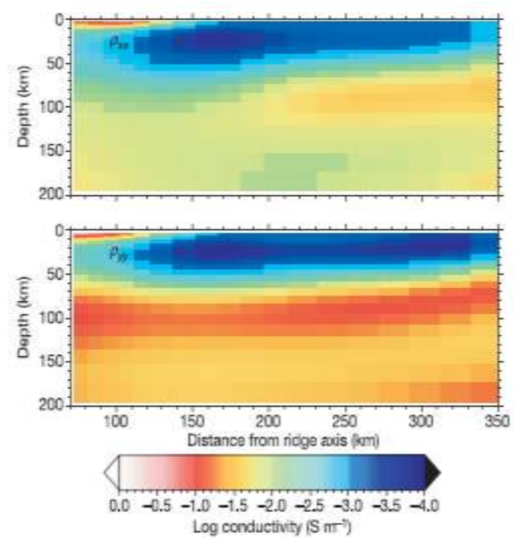
According to the property we focus on (e.g., ***temperature, composition, Vs, Vp, anisotropy, electrical conductivity…****) there are many possible “****LABs****” (e.g. Eaton 2009):*



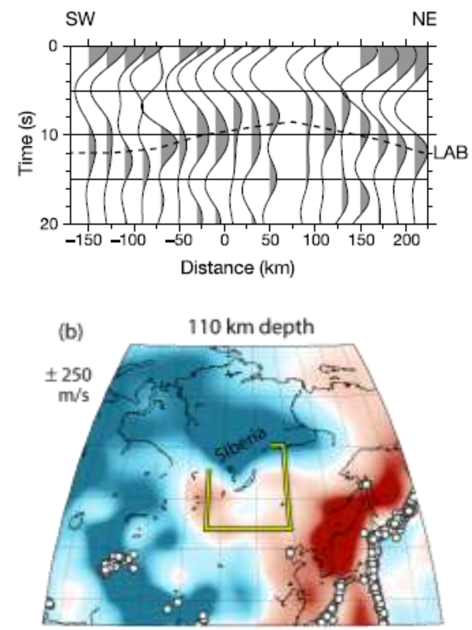
Thermal LAB



Geochemical/ petrological LAB



Electric LAB

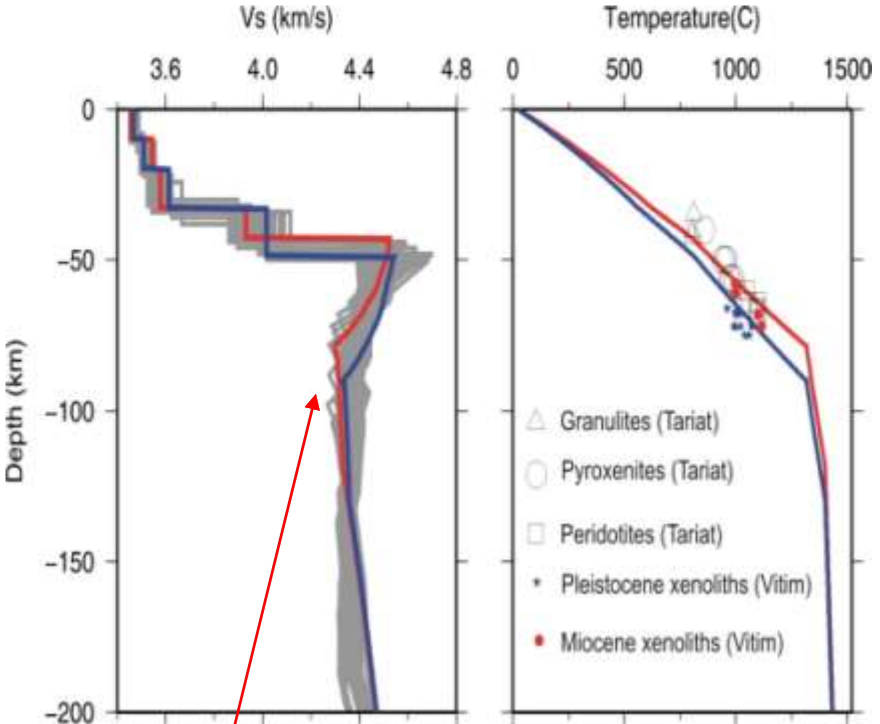


Seismic LAB

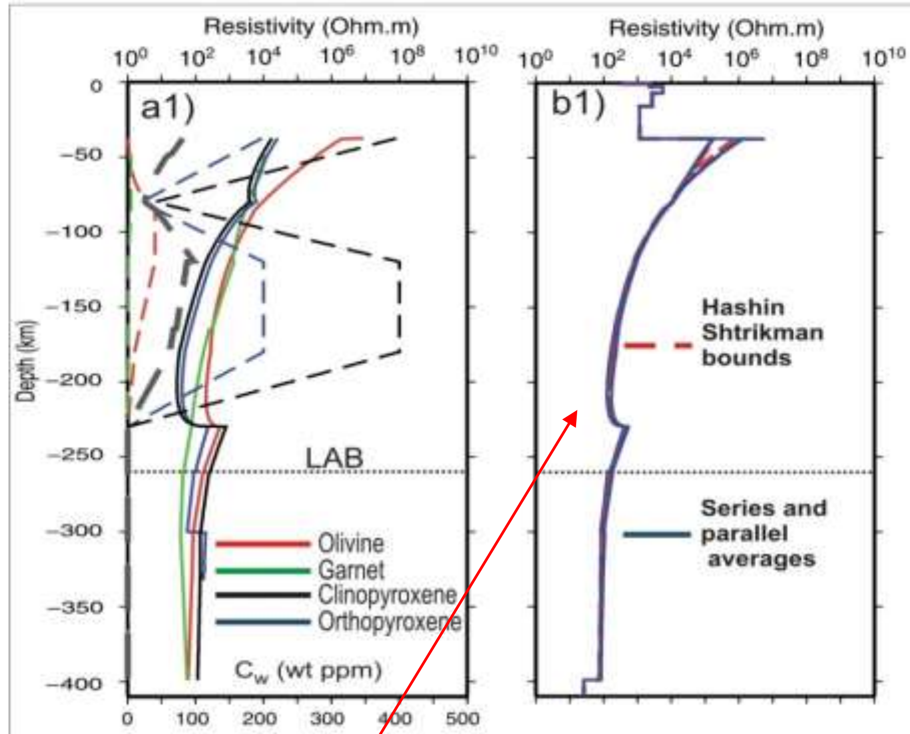
Why integrated modelling...?

*Ultimately most of the **LAB** definitions depend upon **temperature/pressure and composition***

Surface waves



Magnetotelluric



Low Velocity Zone → ***Temperature+Pressure+ Attenuation***

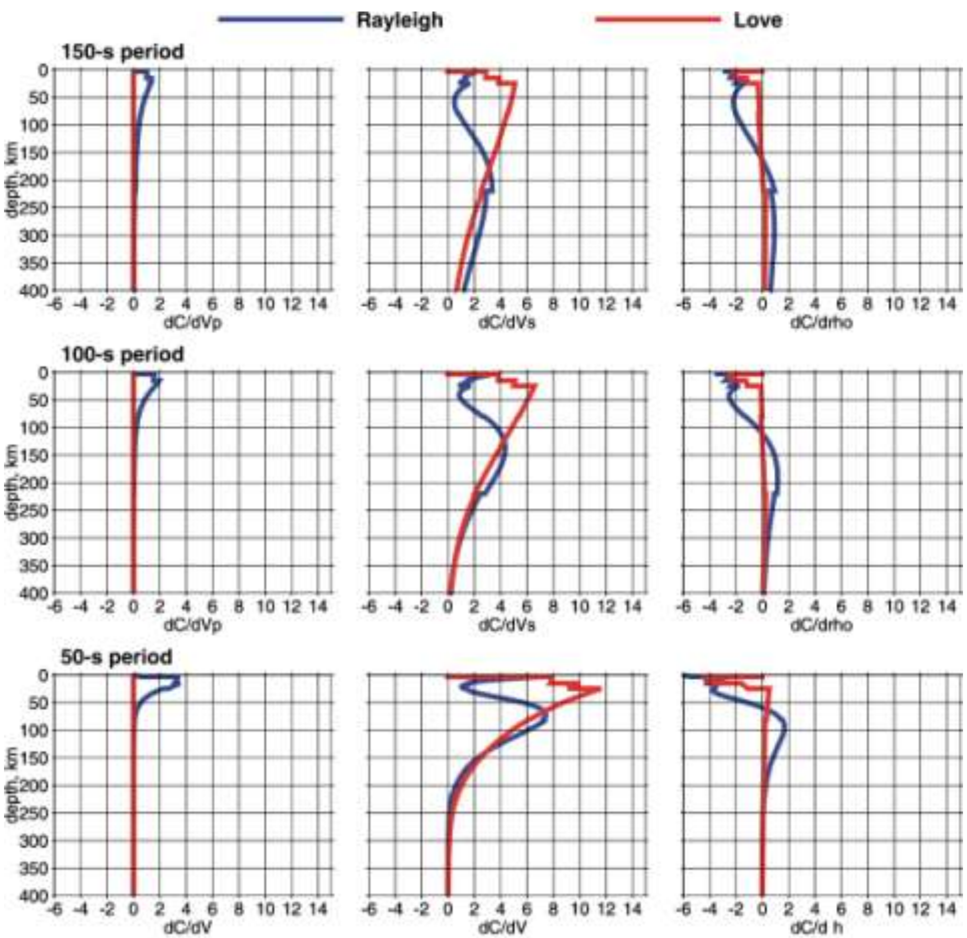
Low Resistivity Zone → ***Temperature+Water***

→ Unify LAB's criteria

Why integrated modelling...?

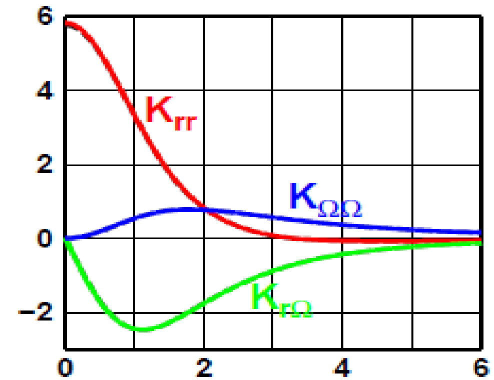
Geophysical observables have different sensitivities to T, C variations (via seismic velocities, densities, conductivity…)

Surface waves sensitivity kernels

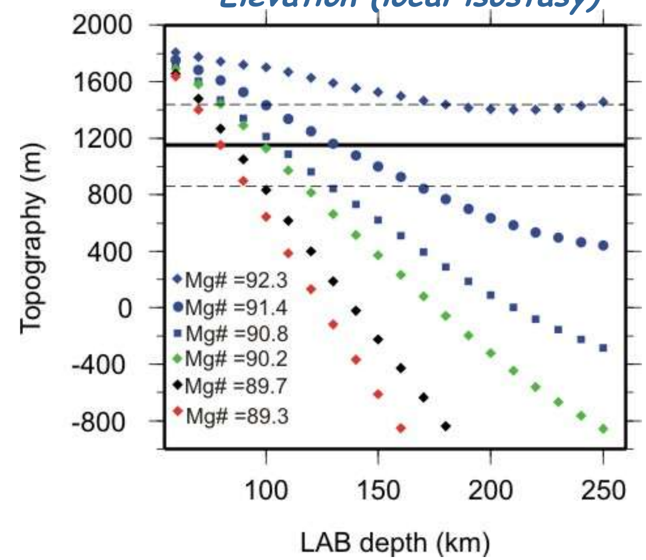


Vp *Vs* *density*

Gravity gradients kernels @ 255 km

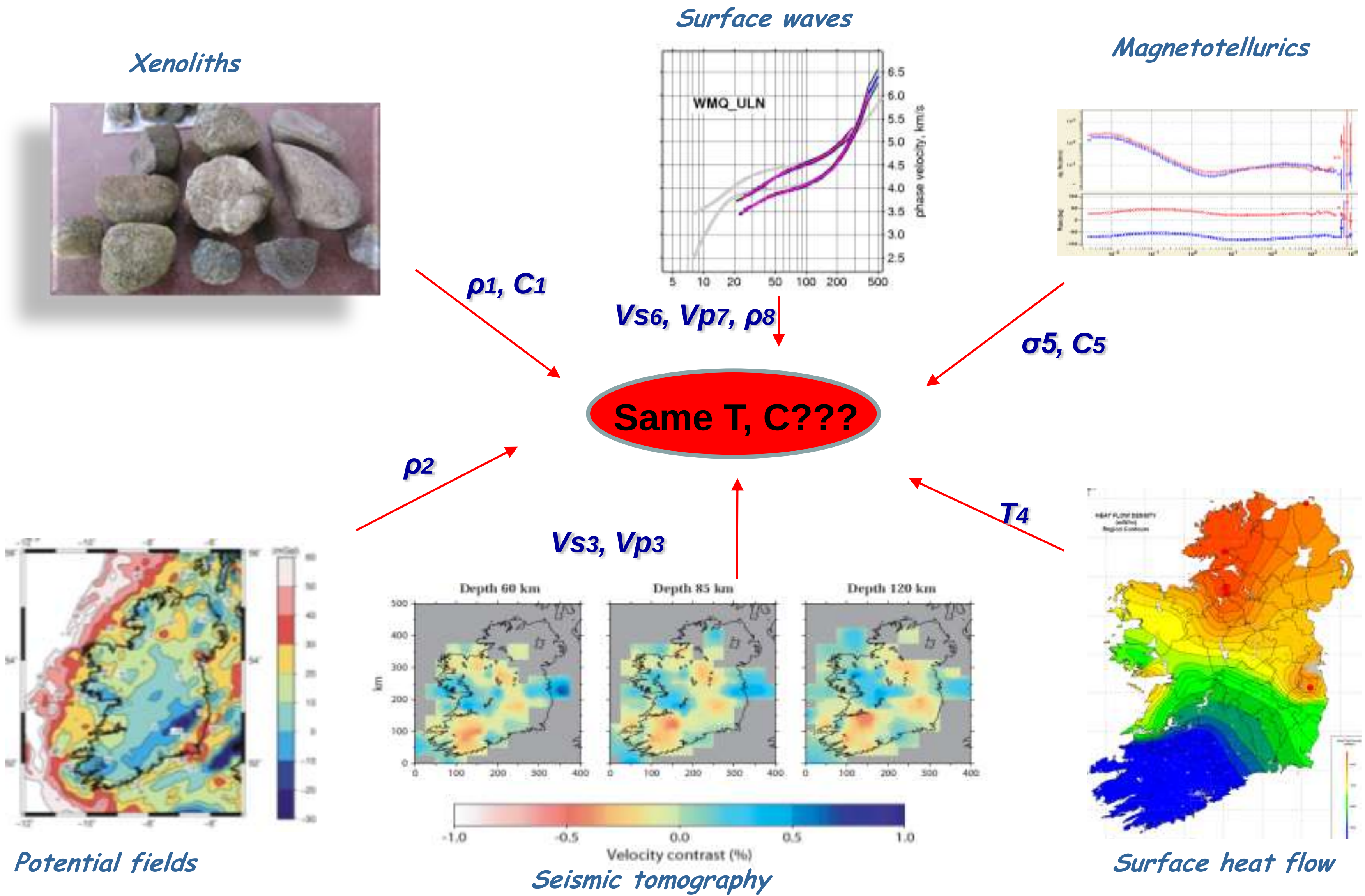


Elevation (local isostasy)



Why integrated modelling...?

Modelling all the observables together **avoids (*some*) inconsistencies** given the non-uniqueness of the physical problem at hand



*Ultimately most of the **LAB** definitions depend upon **temperature**/pressure and composition*

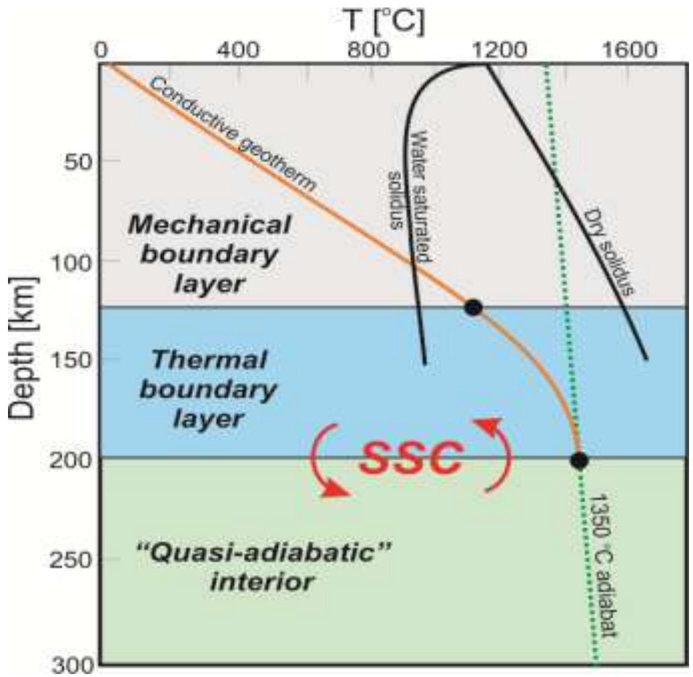
Heat transport equation:

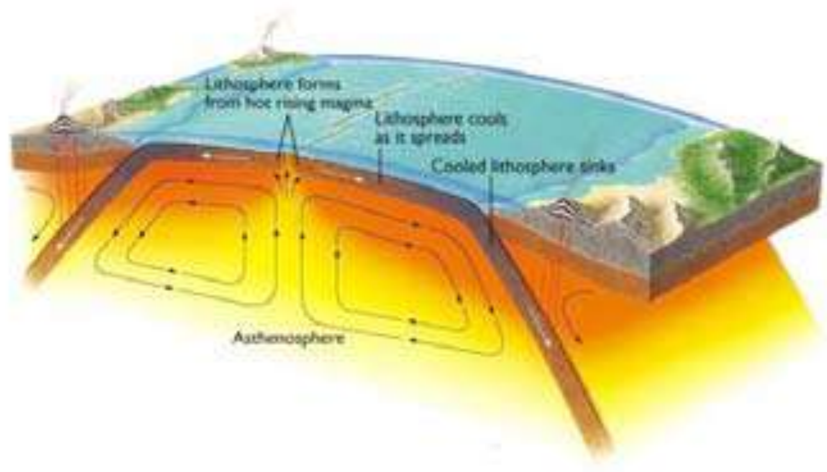
$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + H - \rho c_p \vec{u} \cdot \nabla T$$

Lithosphere: conductive mantle

Steady-state conduction equation: dT/dt=0 and U=0→Diffusion PDE

$$\nabla \cdot [k(\vec{x}, T, P) \nabla T(\vec{x})] = -H(\vec{x})$$





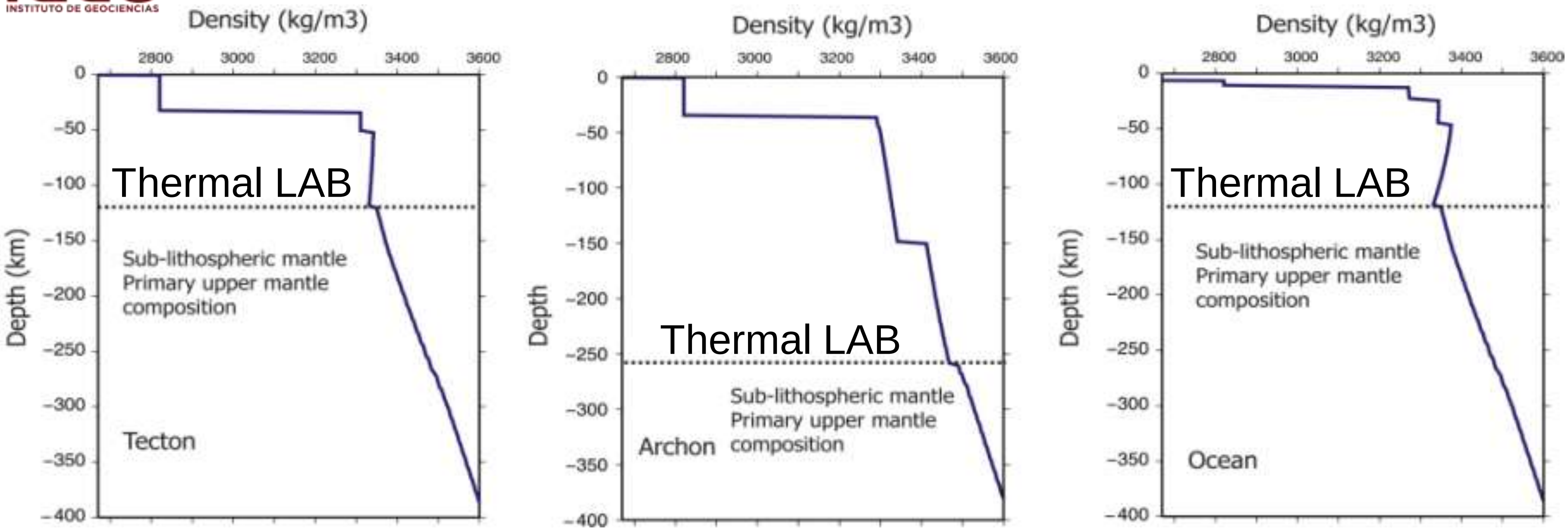
Sub-Lithosphere: mantle convection

Convection in the mantle (i.e. no heat interexchange with the surroundings). Fast heat transport mechanism compared to conduction

$$\left(\frac{\partial T}{\partial r} \right)_S = \frac{T \alpha g}{c_P}$$

Adiabatic gradient: typically 0.45-0.6 K/km in the uppermost mantle

Ultimately most of the **LAB** definitions depend upon temperature/pressure and **composition**



	Aver. Archon Gnt. SCLM*	Aver. Kaapvaal Harzburg.	Aver. Tecton Gnt. SCLM *	PUM J79#	PUM MS# *
SiO_2	45.7	45.9	44.5	45.2	45
TiO_2	0.04	0.05	0.14	0.22	0.2
Al_2O_3	0.99	1.3	3.5	4	4.5
Cr_2O_3	0.28	0.34	0.4	0.46	0.38
FeO	6.4	6.0	8.0	7.8	8.1
MnO	0.11	0.1	0.13	0.13	0.14
MgO	45.5	45.5	39.8	38.3	37.8
CaO	0.59	0.5	3.1	3.5	3.6
Na_2O	0.07	0.07	0.24	0.33	0.36
NiO	0.3	0.28	0.26	0.27	0.25
Mg#	92.7	93.1	89.9	89.7	89.3
Cr/(Cr+Al)	0.16	0.27	0.07	0.07	0.05

In the mantle, stable mineral assemblages can be computed by Gibbs free energy minimization either within the system CaO-FeO-MgO-Al2O3-SiO2 (CFMAS) or Na2O-CaO-FeO-MgO-Al2O3-SiO2 (NCFMAS) [*Connolly, 2005*]. Each mantle body is therefore characterized by a specific **major-element composition** (in wt.%), which translates into specific bulk-rock properties.

Why integrated modelling...?

All thermophysical properties (e.g. ***density, seismic velocities, electrical conductivity****) depend on* ***T, P, and Composition***

$$dG = V\,dP - S\,dT + \Sigma_i\, \mu_i\, dX_i$$ + ~~DdE~~

Thermodynamic equilibrium (T>500 C)

$$V = \left(\frac{\partial \mathcal{G}}{\partial P}\right)_T \qquad V\alpha = -\left(\frac{\partial \mathcal{S}}{\partial P}\right)_T = \left(\frac{\partial^2 \mathcal{G}}{\partial P \partial T}\right) \qquad C_P = -T\left(\frac{\partial^2 \mathcal{G}}{\partial T^2}\right)_P \qquad c_{ijkl} = \frac{1}{V}\left(\frac{\partial^2 \mathcal{G}}{\partial S_{ij} S_{kl}}\right)_{P,T}$$

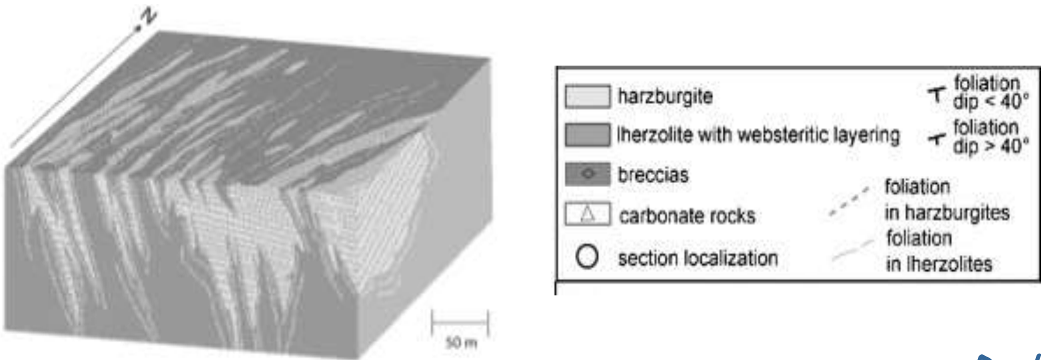
$$\sigma = \sigma_0 \exp\left(\frac{-\Delta H(X_{Fe}, P)}{k_B T}\right) + f(C_w)\exp\left(\frac{-\Delta H_{wet}(C_w)}{k_B T}\right) + \sigma_{0i}\exp\left(\frac{-\Delta H_i}{k_B T}\right)$$

- First term: small polaron (electron hopping between ferric Fe3+ and ferrous Fe2+ ions) at T<1300 ºC
- Second term: Proton conduction (H+ bound to structural O atoms)
- Third term: Ionic conduction (Mg vacancies) T>1300 ºC

→ connect laboratory studies & thermodynamics with geophysics

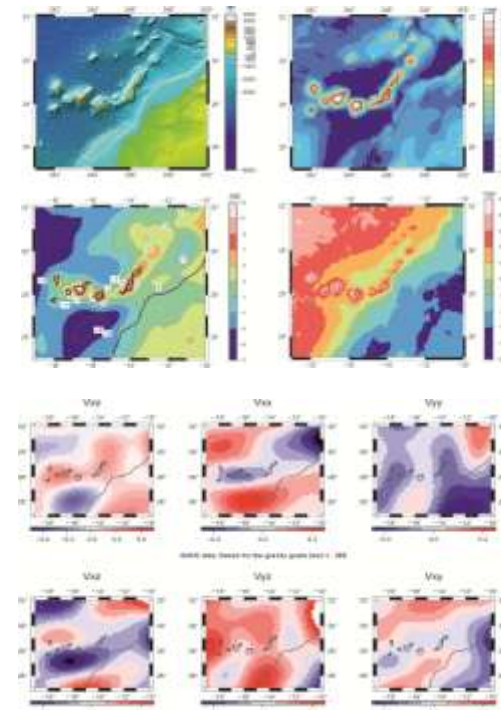
Why integrated modelling...?

Representativeness of observed mantle samples (xenoliths, peridotite massifs etc..) on the lithospheric scale



Forward modeling

Geophysical data



Depleted

Depleted +metasomatised

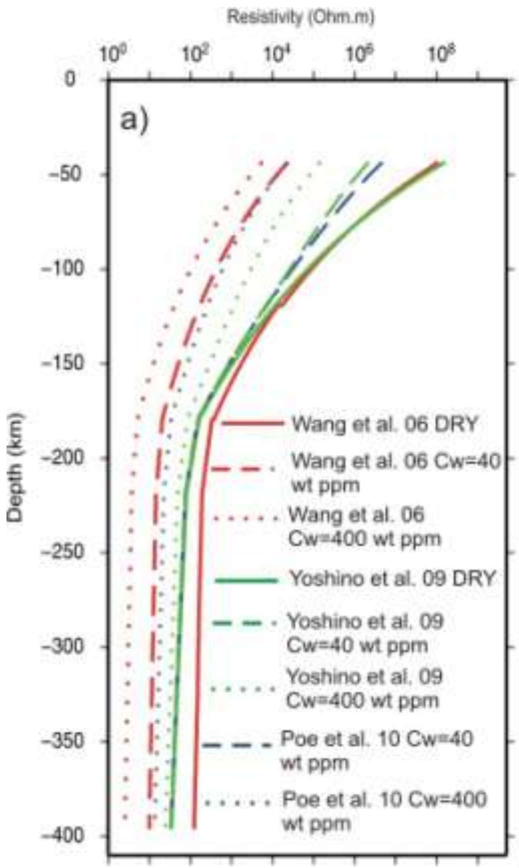
	1) Av. Harz. Lanzarote (wt%)[a]	2) Av. HEXO Tenerife (wt%)[b]	3) Av. Harz. La Palma av. (wt%)[c]	4) Av. HLCO Tenerife (wt%)[b]	5) Av. Ocean floor peridot. (wt%)[d]	6) Av. Middle Atlas (wt%)[e]
SiO_2	43.78	43.32	43.07	42.14	45.09	43.48
Al_2O_3	0.7	0.61	0.53	0.73	2.33	2.38
FeO	7.79	8.04	8.43	8.8	8.4	8
MgO	46.1	45.31	45.19	44.14	41.23	42.6
CaO	0.6	0.81	0.68	1.68	1.32	2.83
Na_2O	0.1	0.14	0.17	0.18	0.23	0.24
Mg#	91.34	90.96	90.53	89.94	89.7	90.47

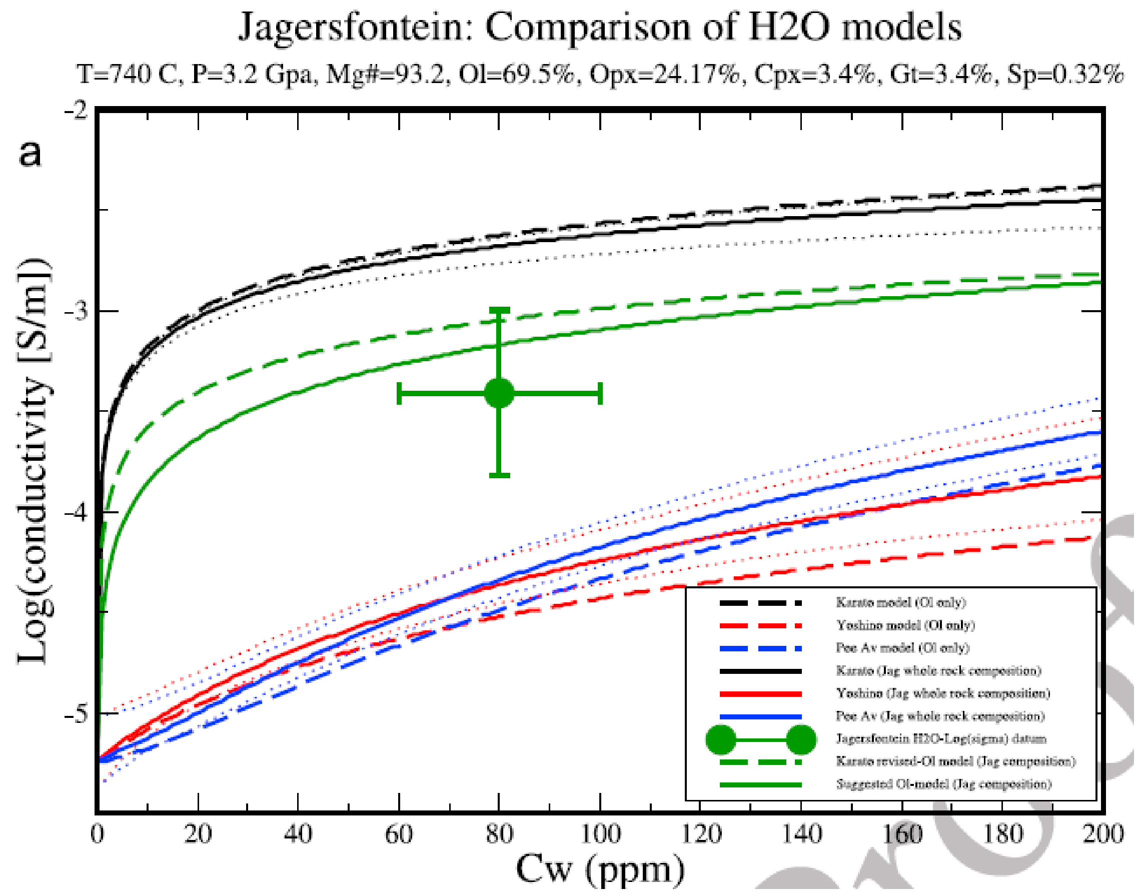
Mantle Depletion (partial melting)

Mantle metasomatism (refertilization)

Why integrated modelling...?

olivine





For olivine there are two models for proton conduction based on lab studies:

$$\sigma_P = \sigma_{0p} C_w \exp\left(\frac{-\left(\Delta H_0 - \alpha C_w^{1/3}\right)}{k_B T}\right)$$

→ *e.g. Yoshino et al., 09; Manthilake et al., 09 ; Poe et al., 10*

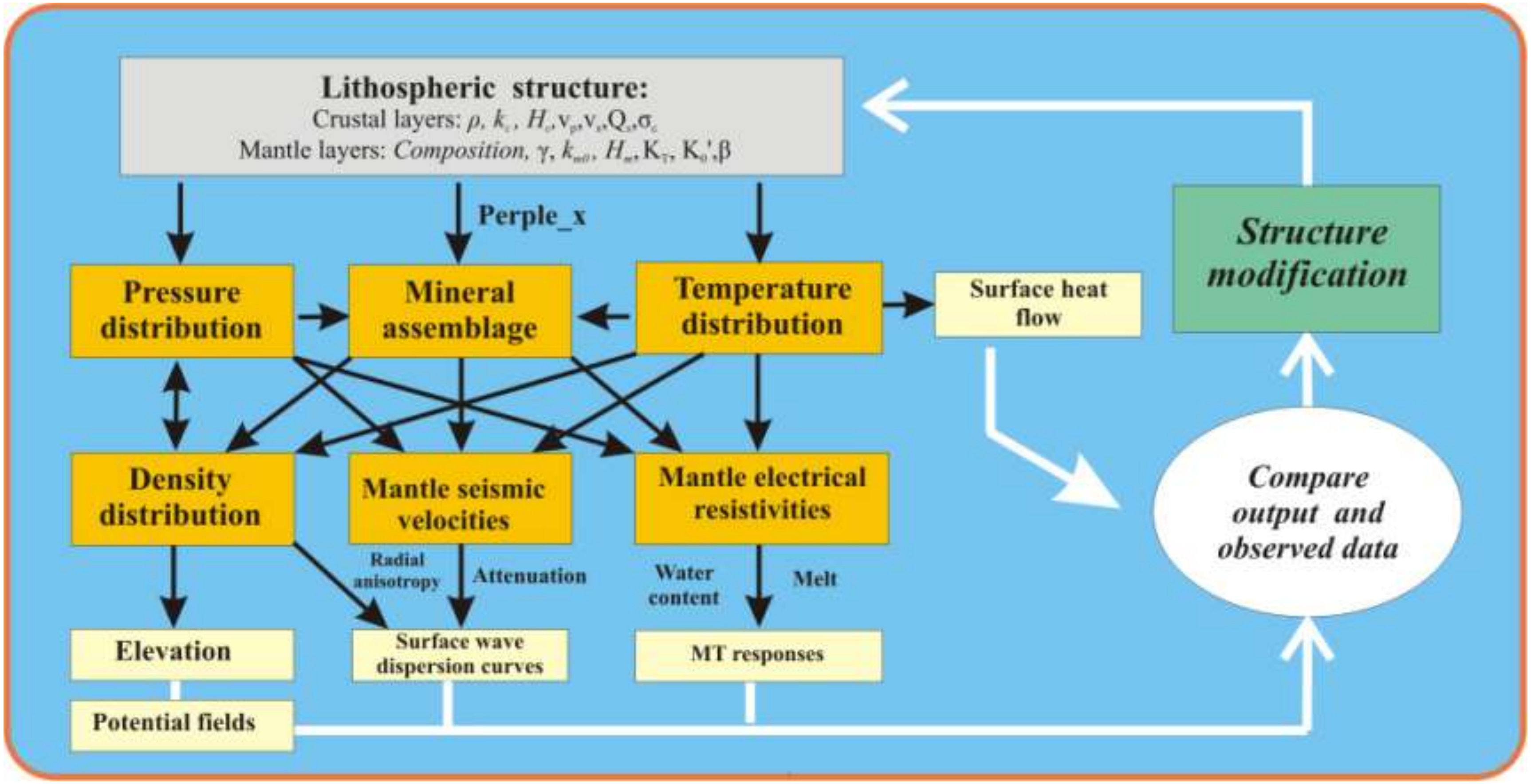
$$\sigma_P = A C_w^r \exp\left(\frac{-\Delta H_{wet}}{k_B T}\right)$$

→ *e.g. Wang et al., 06; Dai and Karato 09*

→ *Calibrate lab studies with geophysics*

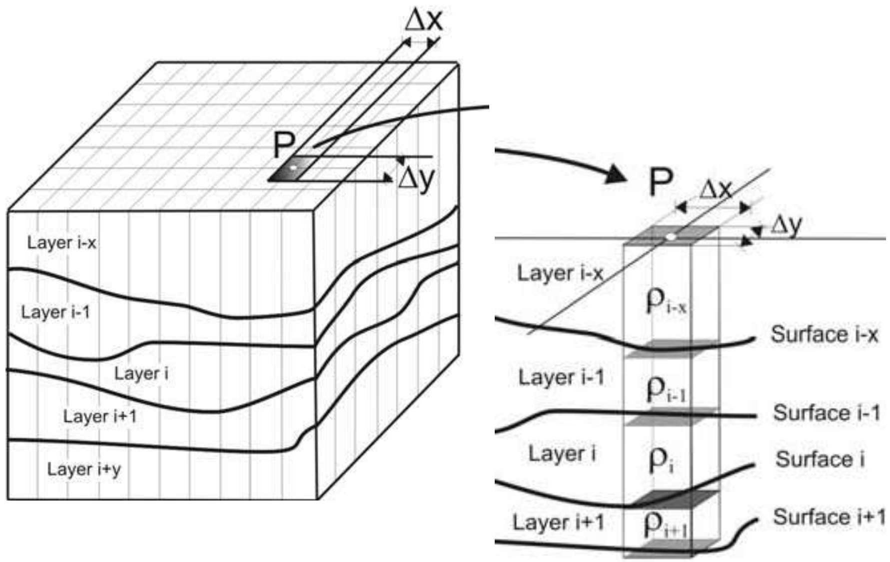
Forward modelling: trial and error

Lithospheric model→Observables (e.g., topography, potential fields, seismic data, MT…)

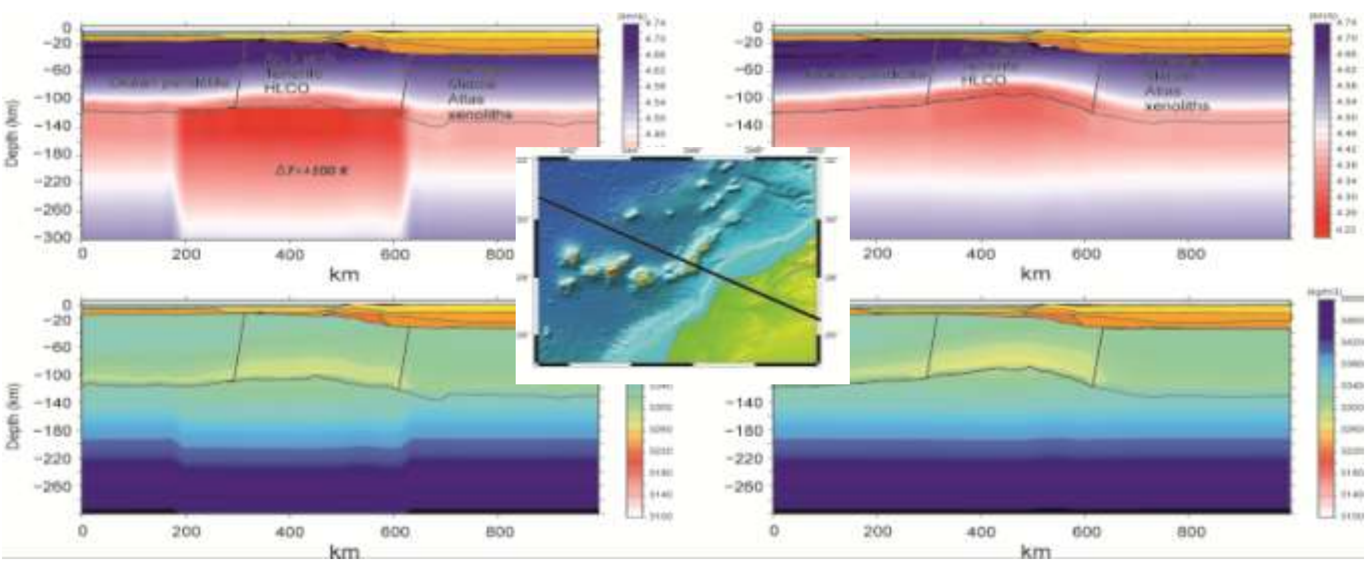


All necessary files containing thermodynamic information can be generated with the freely available software **Perple_X** [www.perplex.ethz.ch, *Connolly, 2005*].
Forward codes **LitMod** (1D,2D,3D) for integrated modelling available at [http://eps.mq.edu.au/~jafonso/Software1.htm , *Afonso et al., 2008; Fullea et al, 2009*].

Forward modelling: advantages



*High spatial resolution (fine grids) depending on computational power available



*Exploratory nature, hypothesis testing

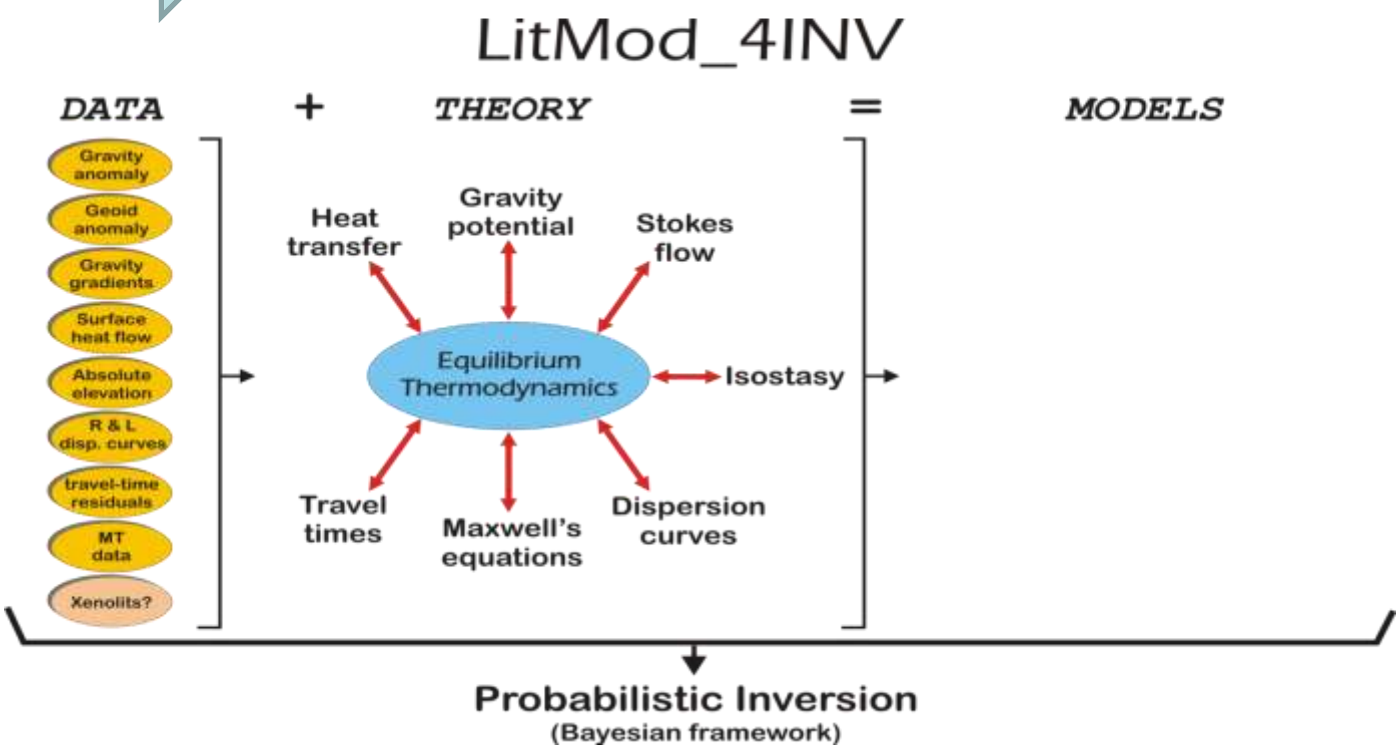
Forward modelling: disadvantages

*Requires a priori/complementary info

*Huge (potential) parameter space, time demanding task

*Possible bias from the modeller's prejudices/background

Inversion "version" of LitMod??

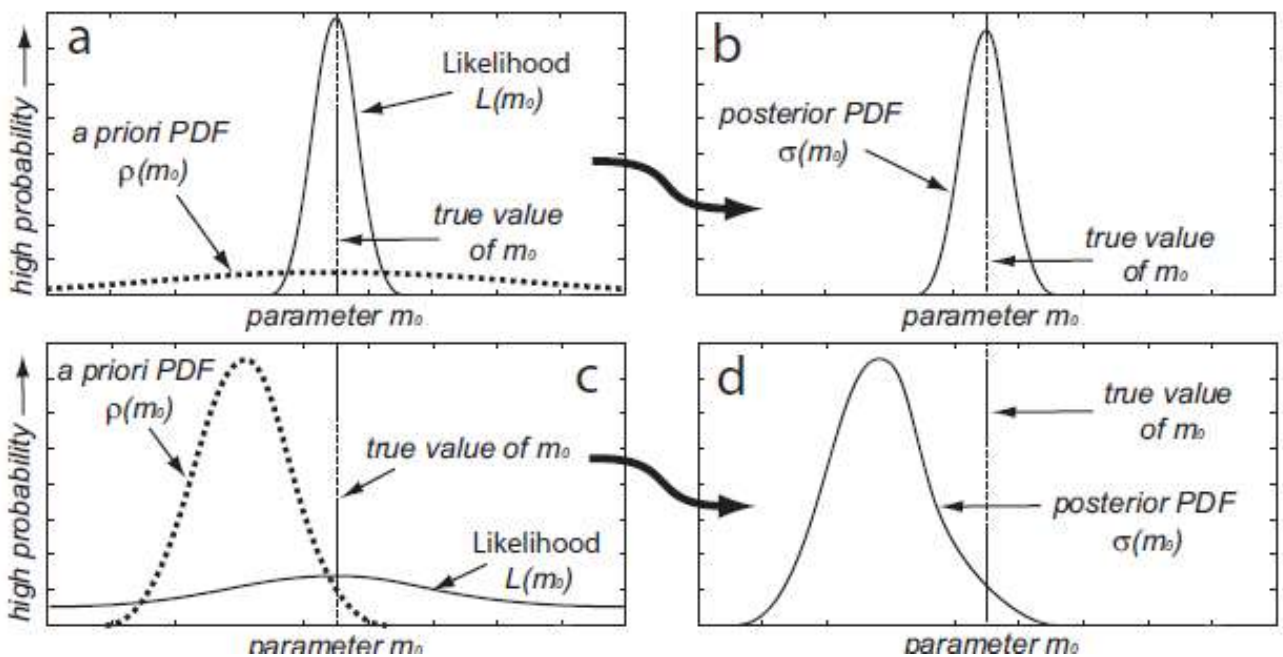


Afonso et al. I and II JGR (2013).

Probabilistic non-linear inversion

*Looking for T and C (5 oxides+water) at every model node
*Typical forward model: 50x50x200 (5E5) nodes→ 5E5*7 param/node=3.5 millions of parameters!!
*Systematic brute-force inversion scheme not affordable
* The physical problem is highly non-linear
*A good control on prior PDF **ρ(m)** (a priori info) and likelihood **L(m)** (observational and theoretical uncertainties, covariance matrix) is essential.

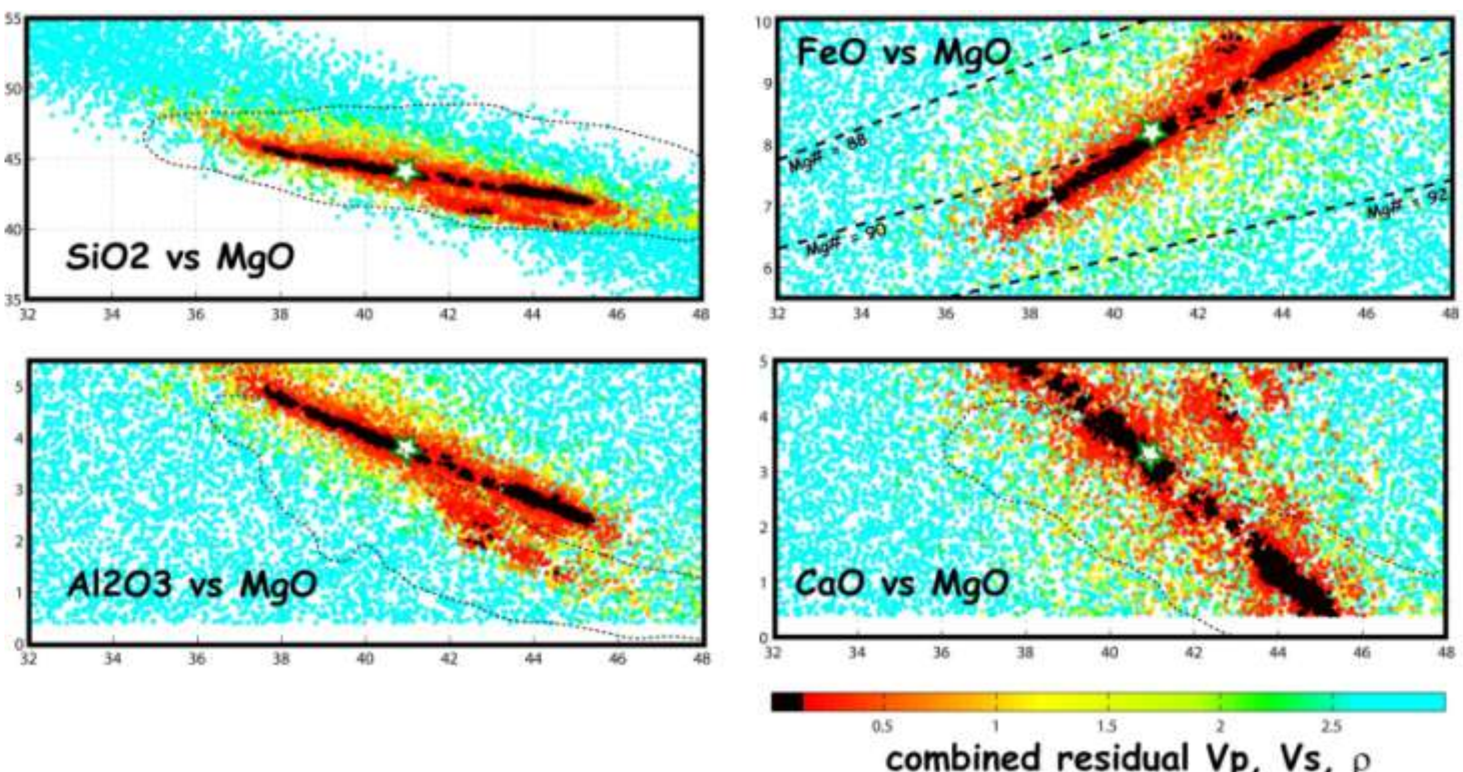
$$\sigma(\mathbf{m}) = k\rho(\mathbf{m})L(\mathbf{m}) \qquad L(\mathbf{m}) \propto \exp\left\{-\frac{1}{2}[g(\mathbf{m})-\mathbf{d}_{\mathrm{obs}}]^T C_D^{-1}[g(\mathbf{m})-\mathbf{d}_{\mathrm{obs}}]\right\}$$



Probabilistic non-linear inversion

* Trade-offs between T and C
* T has a greater effect than C in most of the observables
* Non uniqueness of compositional field (worse in the lithosphere than in the sublithosphere)

$$\sigma(\mathbf{m}) = k\rho(\mathbf{m})L(\mathbf{m}) \qquad L(\mathbf{m}) \propto \exp\left\{-\frac{1}{2}[g(\mathbf{m})-\mathbf{d}_{\text{obs}}]^T C_D^{-1}[g(\mathbf{m})-\mathbf{d}_{\text{obs}}]\right\}$$



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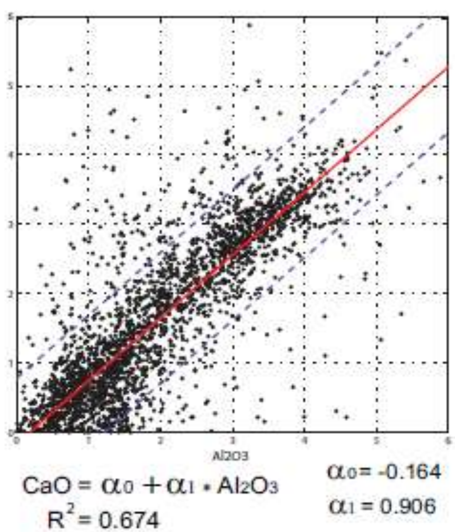
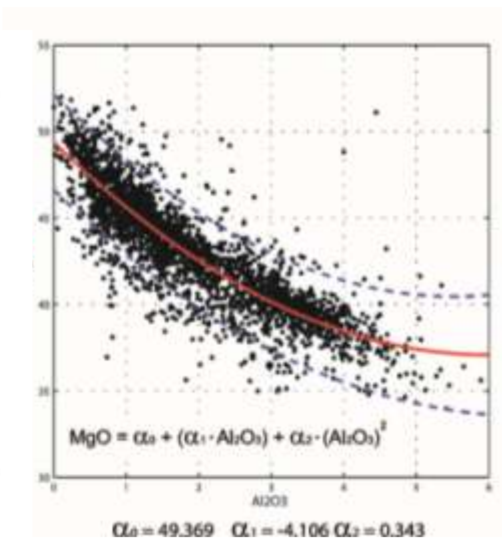
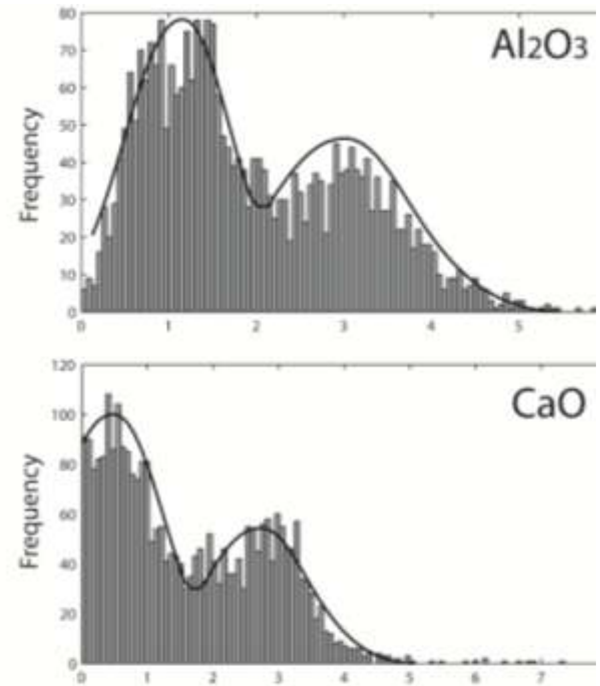
Defining prior PDF ρ(m)

* A priori petrological data base (>2900 samples from xenoliths, perid. Massifs and ophiolites)
* Correlation between oxides (Al2O3 and FeO as independent C param.), regardless of tectonic age or facies.
* Possible bias in database (e.g. double peaks) due to
* Wide Al2O3 and FeO ranges (>95% of natural variability) with uniform probability density

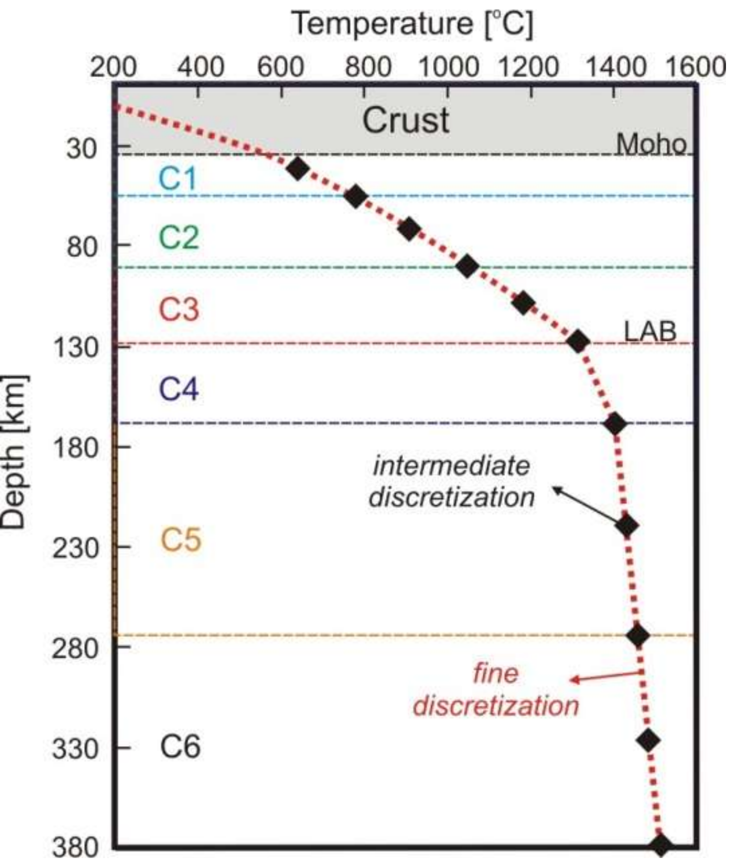




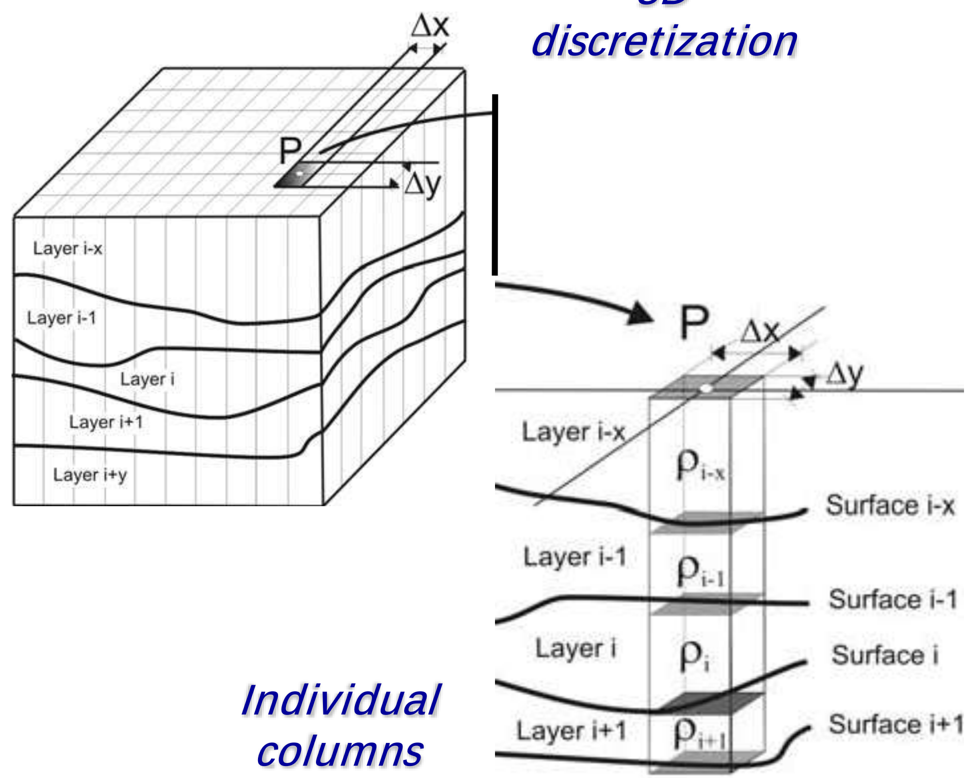


Reducing the parameter space

* Lower resolution: 6 compositional layers and 12 "thermodynamic nodes" (vs 200 vertical nodes in fwd. models)
* Split the 3D problem into 1D columns (for 1D data)→first order PDF's used as priors in the full 3D inversion
* PDF's sampled via MCMC simulation using Metropolis-Hastings algorithm



3D discretization



Individual columns

Method I

First Part

(search & appraisal in 1D)

Input

* *Dispersion curves*
* *1D geoid anomaly*
* *xenolith data*
* *Vp structure*
* *elevation*
* *MT data*
* *surface heat flow*

↓

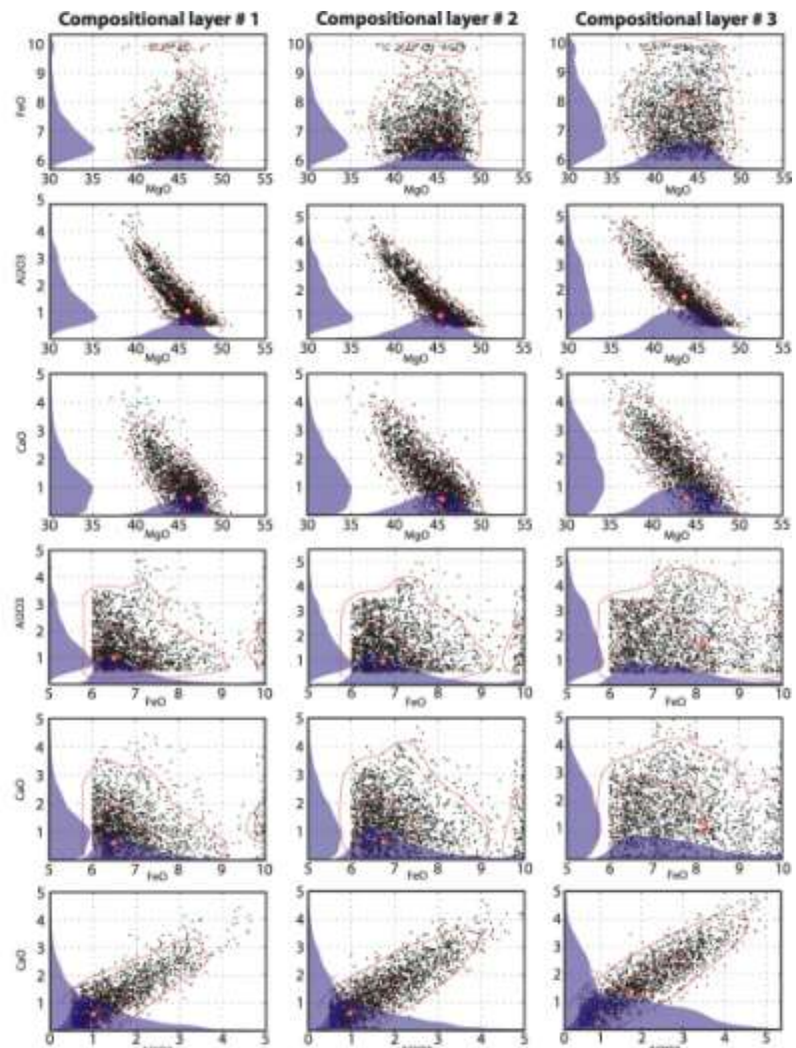
Nonlinear inversion

(***Search*** for acceptable models "column by column" and their PDFs using NA)

↓

Output

(**PDFs for all parameters in all individual columns**)

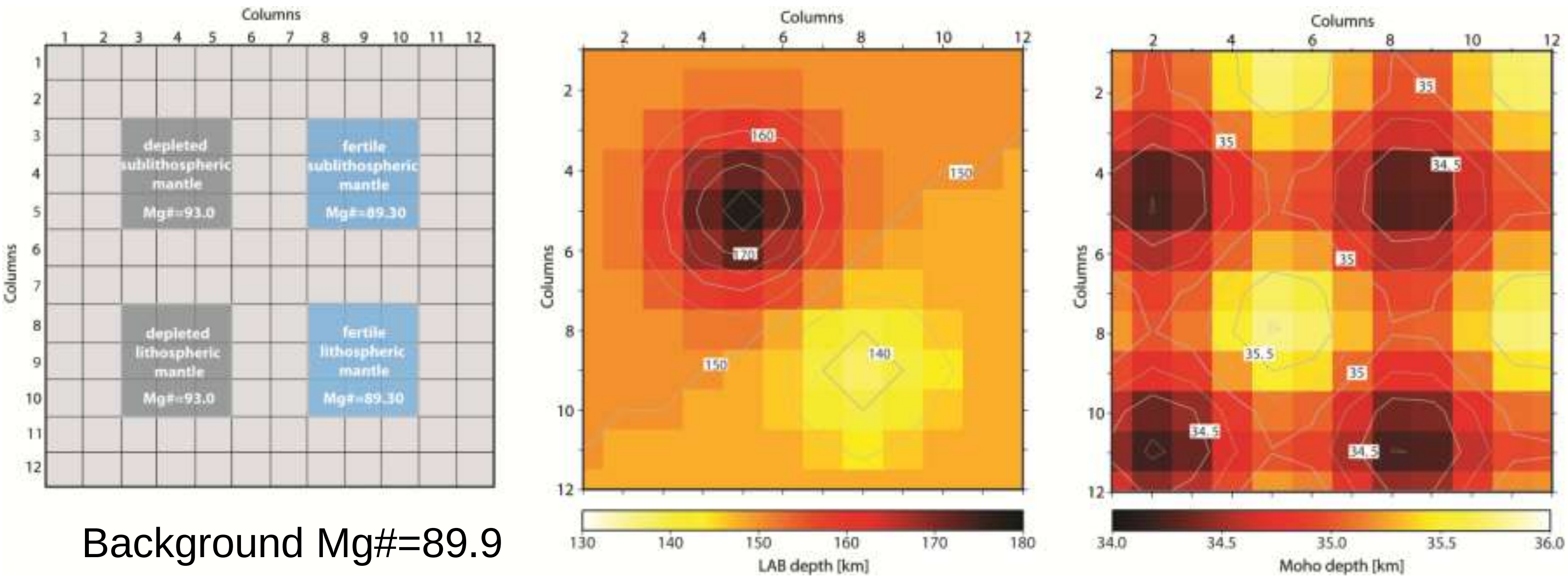


1D Search focused in T: average lithospheric/sub-lithospheric C, dT>200 K

1D search focused on C: 6 compositional layers using LAB posterior PDF

Synthetic test

*4 compositional domains + laterally varying LAB and Moho →its forward responses+noise serve as input for the inversion

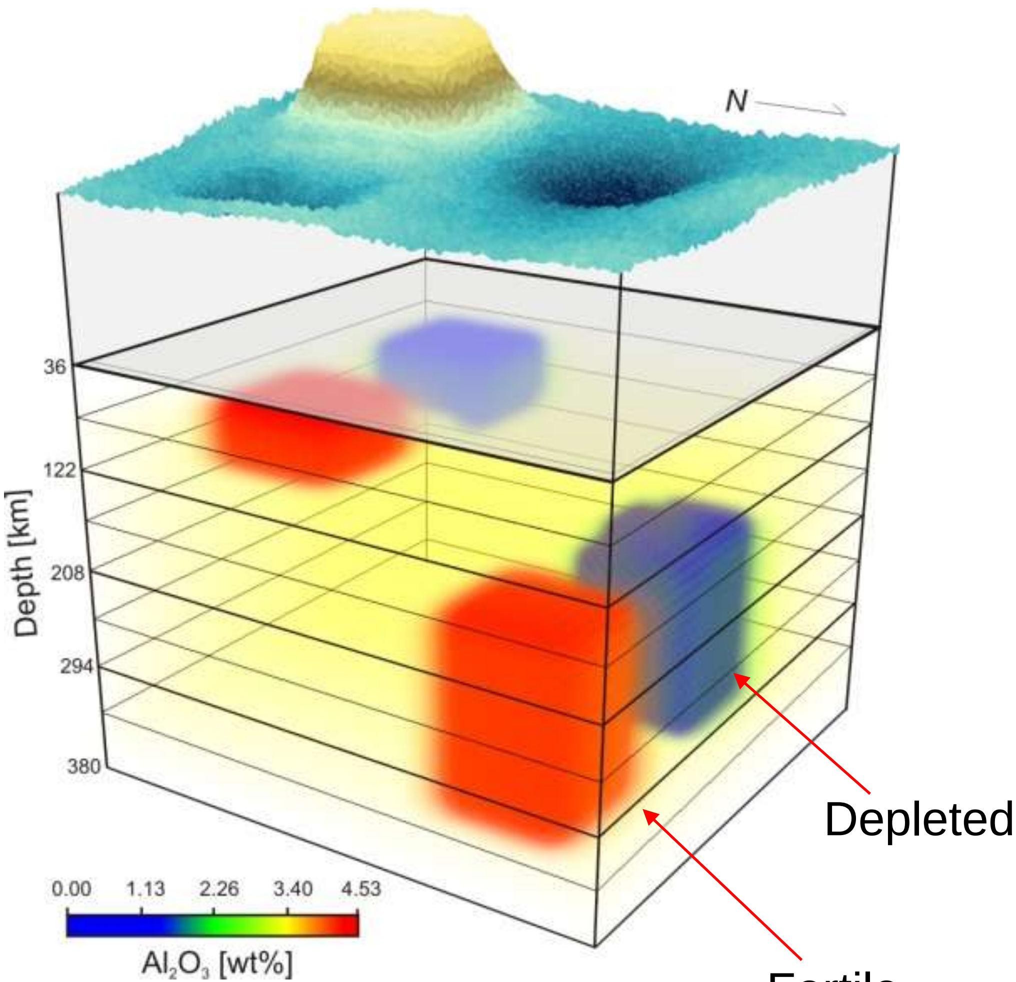


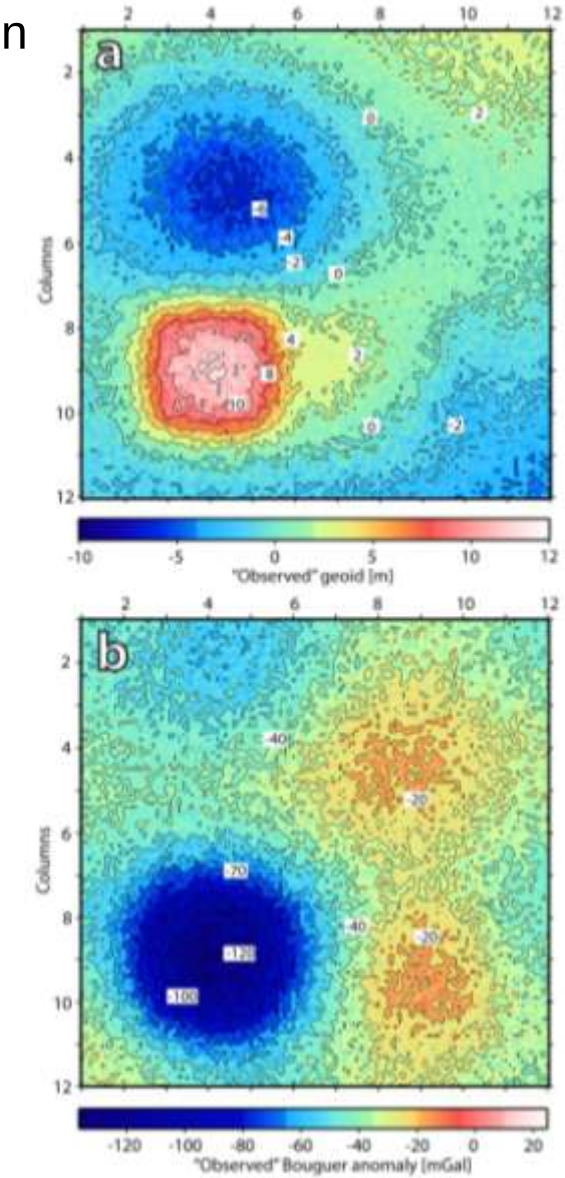
Background Mg#=89.9

Domains **LAB** **Moho**

Synthetic test

Inputs (synthetic fordward+noise) used in the inversion



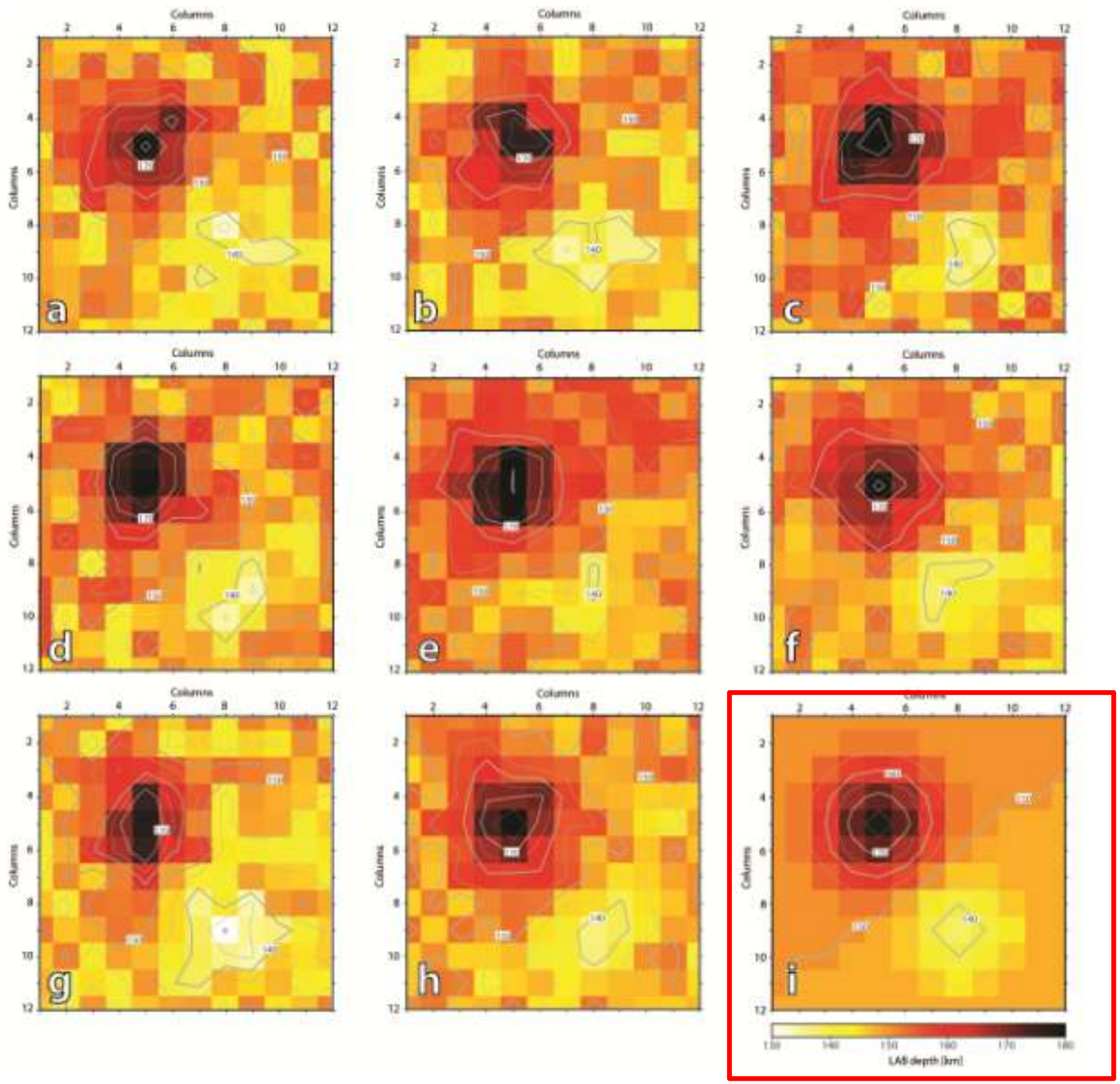


Synthetic test

Results for LAB geometry

Mean models of 8 random ensembles with 500 samples each taken from the total posterior.

Regular and smooth posterior PDF→ averaging is meaningful

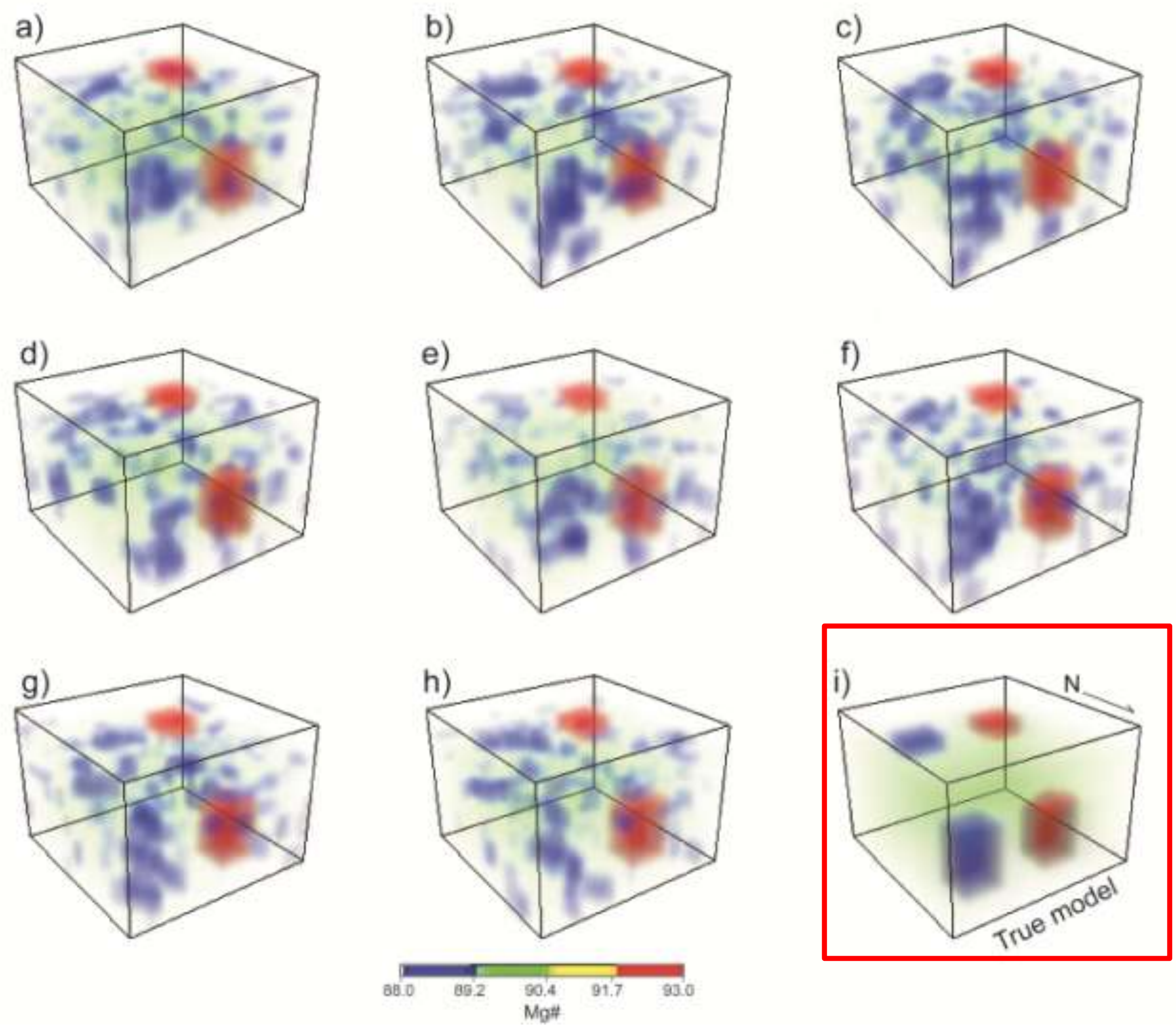


Synthetic test

Mean models of 8 random ensembles with 500 samples each taken from the total posterior

Depleted domains (high Mg#) are recovered, fertile ones (low Mg#) are blurred

Results for Mg#

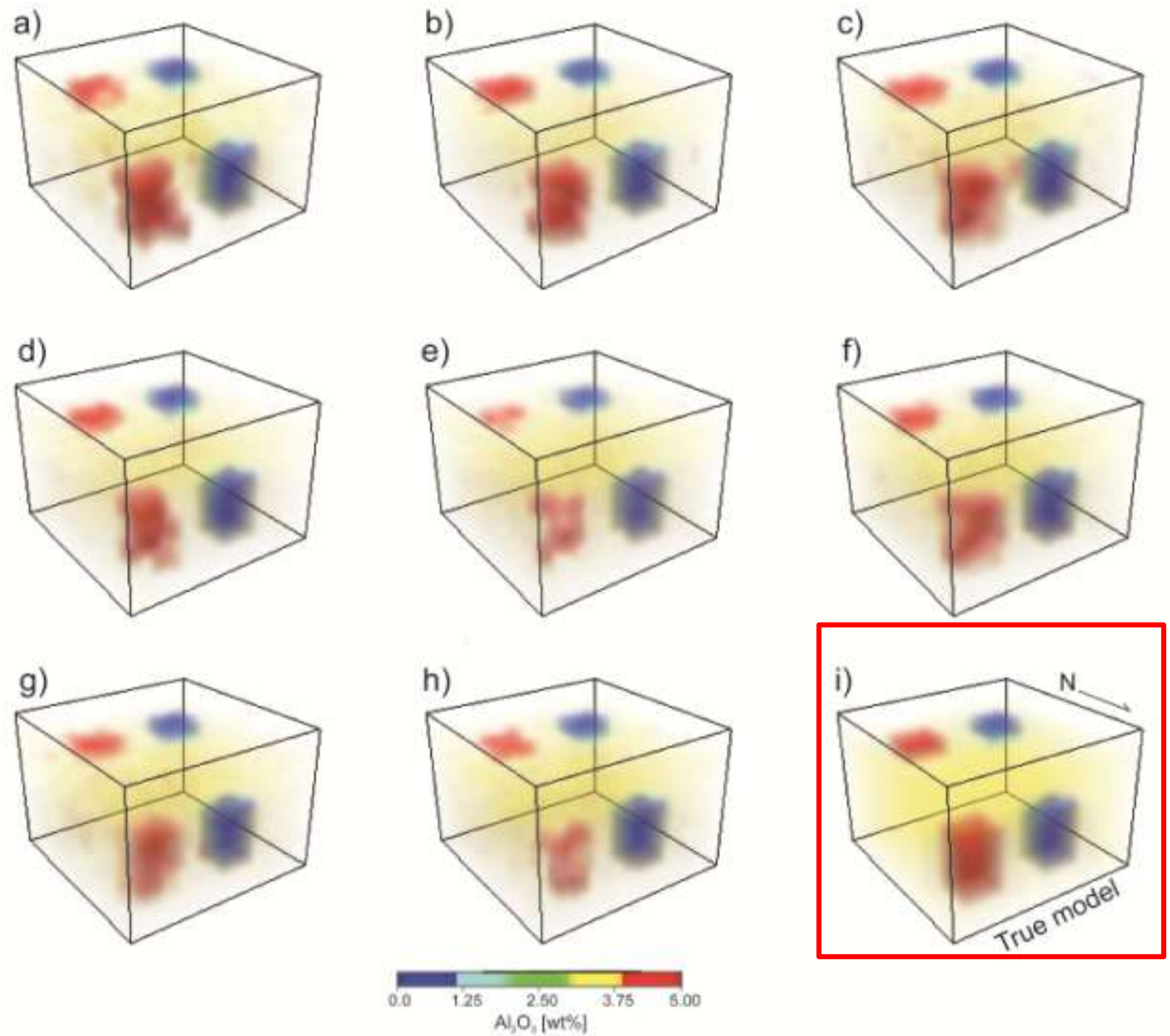


Synthetic test

Results for bulk Al_2O_3

Mean models of 8 random ensembles with 500 samples each taken from the total posterior

Fertile and depleted domains are recovered → Al2O3 is a sensible indicator for compositional end-members



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Internally consistent combination of geophysical observables with different sensitivities to T and C

Integrated modelling: forward vs (and) inversion approaches

Forward model:

- Requires a priori/complementary info

- Huge (potential) parameter space, time demanding task

- Possible bias from the modeller's prejudices/background

+ Relatively fast (seconds-minutes)

+ High resolution affordable

Probabilistic Inversion:

+ It does not require a priori/complementary info

+ Parameter space (T, C) effectively explored in hours-days

+ No bias from the modeller's prejudices/background

- Relatively low resolution

The best of both worlds…

(1) Inversion *and* (2) detailed forward modelling based on (1) for hypothesis testing

Thank you for your attention!