Thermodynamically constrained joint inversion of seismic refraction, surface elevation and gravity data: Crustal structure and composition in the Porcupine Basin (North-East Atlantic)

D. Molodtsov *, J. Fullea, M. Guerri, B. Mather, M. Prada

*Dublin Institute for Advanced Studies, School of Cosmic Physics, Geophysics Section, * mitya@cp.dias.ie*

DIAS Institiúid Ard-Léinn Bhaile Átha Cliath | Dublin Institute for Advanced Studies

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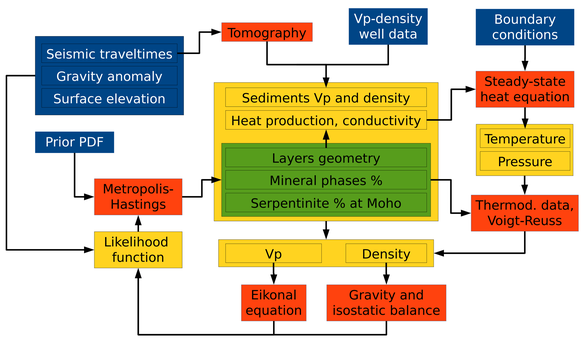
Summary

The Porcupine Basin is a failed rift offshore SW of Ireland, formed in response to several rifting and subsidence phases during the Late Paleozoic to Cenozoic. Information on the composition of the crystalline crust and the uppermost mantle is crucial for better understanding of the tectono-magmatic processes involved in the formation of the Porcupine Basin. To infer this information we develop probabilistic joint inversion of active-source seismic traveltimes, surface elevation and gravity data.

The unknowns of the inverse problem are the proportions of metastable mineral phases within the crust, geometry of the Moho, interfaces between different petrologies and serpentinite content in the uppermost mantle. For a given petrology, elastic moduli and density of the composite are computed as functions of pressure and temperature. This petrological forward problem provides seismic velocities and density, from which geophysical forward solvers predict first-arrival traveltimes, free-air gravity anomaly and bathymetry. In view of strong nonlinearity and nonuniqueness of the inverse problem we apply Markov chain Monte Carlo (MCMC) algorithm with Parallel Tempering to sample the posterior probability density function (PDF) of the model parameters. Posterior PDF appears to be multimodal and is further analyzed using Gaussian mixture model.

Here, we present the results of testing of our inversion framework on synthetic dataset simulating real-world wide-angle seismic experiment in the Porcupine Basin.

Inversion framework



Forward problems:

- Velocity and density calculations – Perple_X thermodynamic database and Voigt-Reuss averaging, model of serpentinized mantle of Carlson & Miller (2003)
- Steady-state heat equation – finite-differences with SOR solver
- Eikonal equation – solver of Podvin & Lecomte (1991)
- Gravity – analytic expressions to precompute forward operator matrix for regular density grid
- Isostatic balance – formulas of Lachenbruch & Morgan (1990)

Forward solvers are parallelized using OpenMP. To further speed up computations we linearize temperature and pressure problems – we find this reasonable for inversion purposes since the effect of P-T on Vp and density is much weaker compared to that of the composition.

Markov chain Monte Carlo with Parallel Tempering

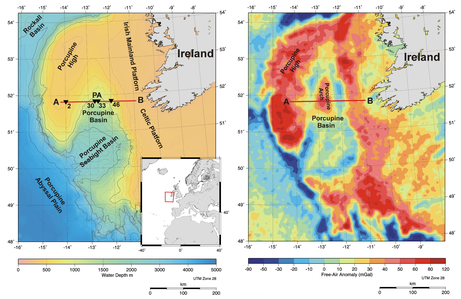
Number of traveltime picks typically exceeds number of gravity and elevation data by one-two orders of magnitude. To account for this, we weight the datasets according to the number of data, so that the likelihood function has the form

$$L(\mathbf{m}) = \exp\left(-\frac{1}{T\sum_i \frac{1}{N_i}} \sum_i \frac{\phi_i(\mathbf{m})}{N_i}\right)$$

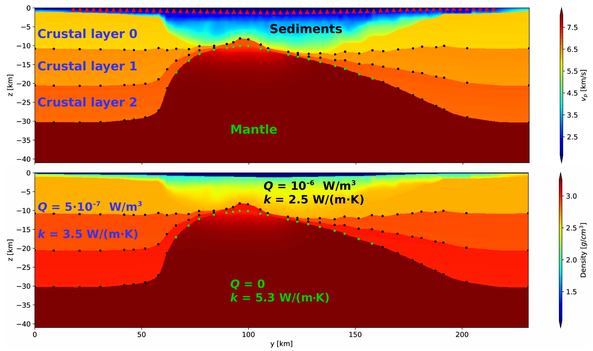
We used uniform prior PDFs with the widest bounds: [0, 100] % for compositional parameters and [0, 40] km for layer thicknesses. There is a natural constraint on the compositions – they must sum up to 100%; additional constraint on the layer thicknesses was that their sum does not exceed 40 km.

In the implementation of the Parallel Tempering algorithm we follow [Sambridge, 2013]: 25% of the Markov chains run at T=1 and the rest are evenly logarithmically distributed along the temperature range (1, 10^7]; at each iteration, interchange of states is proposed to a randomly chosen pair of chains.

Synthetic model



Geographical position of the Leg 4 of the Rockall and Porcupine Irish Deep Seismic (RAPIDS4) wide-angle seismic experiment on bathymetry and satellite free-air gravity anomaly maps [O'Reilly et al., 2006]. The data were acquired in 2002 with 65 OBS. First arrivals are detectable up to ~100 km offsets.



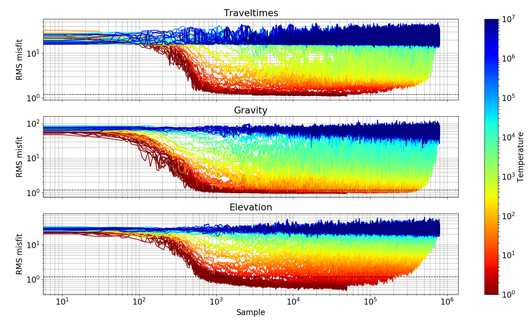
P-wave velocity, density, volumetric heat production Q and standard P-T thermal conductivity k for the synthetic model. OBS positions shown with triangles. Nodes parameterize geometry of the crustal layers, those highlighted in green also parameterize wt% of serpentinite in the mantle.

Model geometry and velocity of sediments are based on the forward-modelling interpretation of the RAPIDS4 data [O'Reilly et al., 2006]; empirical relation [Prada et al., 2018] was used to predict density of sediments.

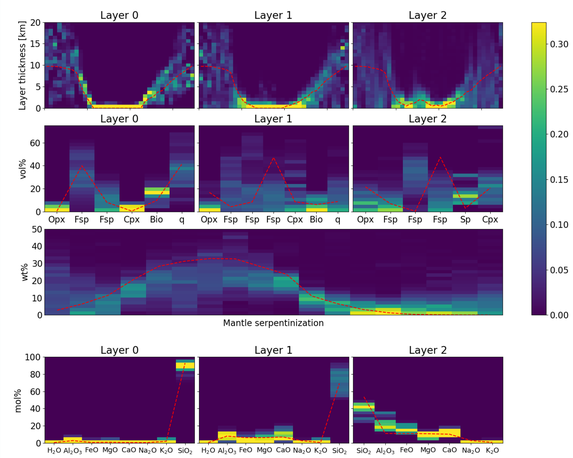
Velocity and density of crustal layers are computed from mineral compositions based on global models of the Earth's crust [Guerri et al., 2015]:

Layer 0		Layer 1		Layer 2	
Phase	**Vol.%**	**Phase**	**Vol.%**	**Phase**	**Vol.%**
Opx	0.49	Opx	16.73	Opx	21.61
Fsp	39.98	Fsp	4.22	Fsp	6.91
Fsp	8.10	Fsp	8.40	Fsp	0.37
Cpx	0.51	Fsp	47.19	Fsp	47.40
Bio	9.74	Cpx	8.56	Sp	2.99
q	41.18	Bio	6.15	Cpx	20.71
		q	8.75		
Opx: 0.43 enstatite 0.57 ferrosilite **Fsp:** 0.06 high albite 0.93 sanidine **Fsp:** 0.61 high albite 0.38 anorthite 0.01 sanidine **Cpx:** 0.09 Ca-tschermaks 0.30 hedenbergite 0.60 diopside **Bio:** 0.41 annite 0.59 phlogopite **q:** quartz		**Opx:** 0.45 enstatite 0.55 ferrosilite **Fsp:** 0.06 high albite 0.94 sanidine **Fsp:** 0.10 high albite 0.89 anorthite **Fsp:** 0.60 high albite 0.39 sanidine **Cpx:** 0.09 Ca-tschermaks 0.28 hedenbergite 0.63 diopside **Bio:** 0.40 annite 0.60 phlogopite **q:** quartz		**Opx:** 0.47 enstatite 0.53 ferrosilite **Fsp:** 0.06 high albite 0.94 sanidine **Fsp:** 0.11 high albite 0.89 anorthite **Fsp:** 0.60 high albite 0.40 anorthite 0.01 sanidine **Sp:** 0.16 spinel 0.84 hercynite **Cpx:** 0.13 Ca-tschermaks 0.24 hedenbergite 0.63 diopside	

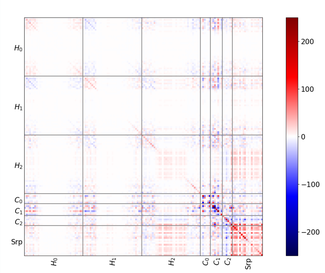
Inversion results



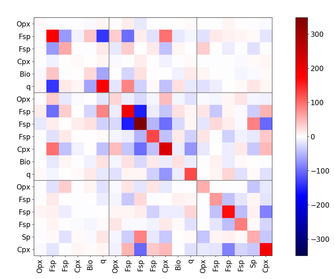
RMS data misfits along the 50 tempered Markov chains. Note that acceptance rate increases with temperature, leading to longer chains. For further analysis we retain samples from 12 chains at T=1 with all RMS below 1.2 (dashed line) – 269083 samples in total.



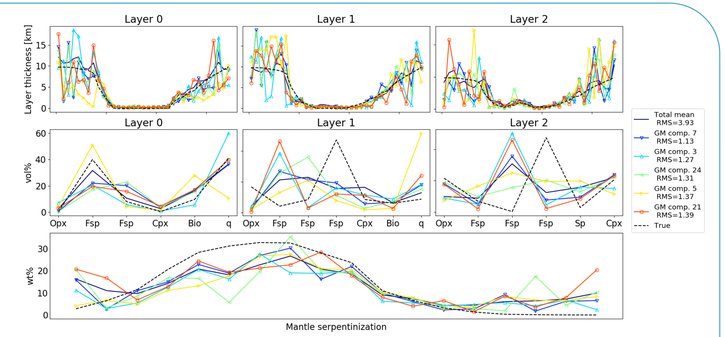
Marginal posterior PDFs of the model parameters and phase compositions decomposed into oxides. True values are indicated by dashed line.



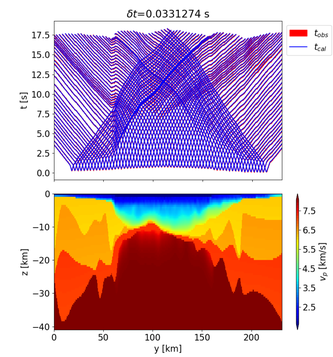
Posterior covariance matrix of the model parameters. $H_{0\text{-}2}$ – layer thicknesses, $C_{0\text{-}2}$ – compositions, Srp – serpentinization.



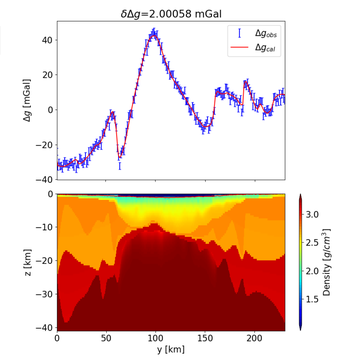
Zoom-in of the crustal composition block.



The sampled distribution was fitted by Gaussian mixture (GM) model using expectation-maximization algorithm. Number of the mixture components was determined as argument of local minimum of the Bayesian information criterion. Here, we show mean models for 5 (out of 27) components with the lowest values of the RMS data misfit. Note the high RMS value for the total mean model, indicating that the sampled PDF is actually multimodal.



P-wave velocity and calculated vs observed first-arrival traveltimes for the mean model of GM component 21.



Density, calculated bathymetry (red line) and calculated vs observed free-air gravity anomaly for the mean model of GM component 21.

Conclusions and future work

- We propose a Bayesian inversion framework to jointly invert active-source seismic, gravity and elevation directly into chemical composition of crystalline crust and upper mantle; thermal parameters can be inverted for as well
- To deal with multimodal PDF, we apply Parallel Tempering MCMC and mixture model to analyze the sampling
- Results of the synthetic test prove feasibility of the proposed approach
- Particularly high uncertainties are associated with geometry at the model flanks and composition of the lower two crustal layers, due to poor ray coverage. To handle this problem, we plan to adapt transdimensional approach
- Results should be improved by using narrower priors
- Adding later P-wave and S-wave arrivals to the inversion, at the expense of increasing computational cost, may reduce the uncertainties

References

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