ÉCOLE DOCTORALE
SCIENCES DE LA TERRE ET DE L'ENVIRONNEMENT
ET PHYSIQUE DE L'UNIVERS, PARIS

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Subject title: Waveform seismic filtering of melt migration beneath the Réunion island with the aid of *ab initio* calculations

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Host lab/ Team: **IPGP- Seismology/CAGE – UMR7154**

Financing: Doctoral contract preferably with teaching assignment

Aim Our proposed PhD research aims to unravel the seismic signatures of subcrustal and upper mantle melts, with a particular focus on the volcanism associated with the Réunion Island. To achieve this, we will employ a cutting-edge combination of seismic modelling, geochemical constraints, and atomistic simulations, which will enable us to develop a robust community tool that can predict seismic signals with remarkable accuracy.

Our approach will involve utilising a wealth of a priori information provided by petrology, geodynamics, and mineral physics to train our predictive model(s), which we will then compare against observed seismic data with a resolution of several kilometres. Through this method, we hope to shed new light on the complex processes governing the melting dynamics in the Earth's mantle and develop a deeper understanding of how these processes lead to the formation of volcanoes. The success of this project could have significant implications for our understanding of the Earth's interior, potentially revolutionising our ability to detect and predict the occurrence of volcanic activity.

Figure 1 is a schematic illustration of this project. Starting from available magma compositions from Réunion, we use *ab initio* modelling to obtain physical properties (density, elasticity) of the magmas. Then we construct plausible 1D/3D geometries beneath the region, and build seismic structures. Simulated seismograms for these models can be compared against observed seismic data to constrain geodynamical/geological structural evolution.

Why does melt matter? Partial melts are observed/imaged everywhere and at every scale in the interior of the Earth. Global tomography suggests hierarchical plume upwelling with repetitive horizontal stagnations (*1*, *2*) while regional and local studies show a similar schema of magma upwelling and magma chambers at smaller scales (*3*, *4*). In a pilot study of waveform seismic filtering (see below), Franken *et al.* (*5*) studied 21 teleseismic records acquired at the land seismometer on Réunion island (RER) in order to constrain 1D partial melt upwelling dynamics, by proposing 210 different geodynamical scenarii. Even with one-seismometer records, our methodology was able to prefer high permeability and high initial temperature while upwelling velocity and porosity were not well constrained. We expect to harmoniously investigate the 1D/3D structural evolution by using more seismic data and by adding more qualitative a priori information from petrology and geochemistry. We build on this study by incorporating geochemical and petrological data from the RHUM-RUM network of ocean-bottom seismometers and from first-hand observations made at the land seismometer at the Réunion observatory. Our project involves performing 3D waveform seismic filtering to constrain better the dynamics of partial melt upwelling in the region.

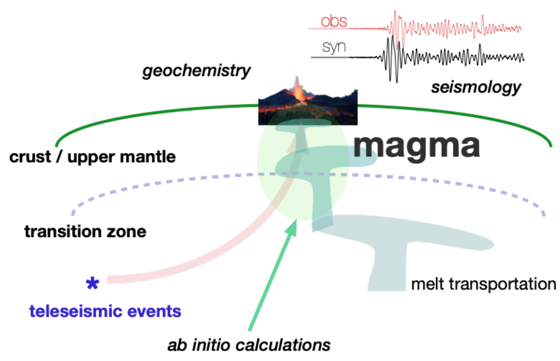

Figure 1: A schematic illustration of this project. Geochemical data are used to predict geometric structural models of magma beneath the Réunion island via *ab initio* calculations. This allows for the computation of synthetic seismograms for teleseismic events to prefer or exclude geodynamical scenarii by comparing them against the observed waveforms. The iterative procedure is aimed at constructing a robust geological-geodynamical model of the structural evolution of melt transportation beneath volcanoes.

Waveform seismic filtering Contrary to the classical quantitative way of collaboration in geosciences that compares seismic tomographic models with geodynamical models, here we have been developing waveform seismic filtering method, a series of forward modelling through various domains that can qualitatively and directly evaluate probabilities of model parameters in geodynamics and in petrology. Here we reconstruct plausible composition and temperature models using different geodynamical/petrological scenarii extrapolated from the surface geochemical observation. We then convert 1D/3D regional models down to the mantle transition zone beneath Réunion island with *ab initio* calculations. We then compute seismic data for every geodynamical and petrological scenario. The advantage of this method is that we have full control of error propagation in each forward modelling (*5*).

Information from *ab initio* calculations Starting from geochemical information harvested at the surface from the erupting lavas, we will use *ab initio* molecular dynamics (AIMD) simulations to characterise the magmas in the shallow Earth. One of the key benefits of AIMD is that they provide a detailed, atomistic-level understanding of a mineralogical system. This allows us to study the behaviour of individual atoms, molecules, and chemical species and to observe the molecular-level interactions that drive the behaviour of the system as a whole (*6*). In many cases, this level of detail is not accessible through experimental methods, making MD an important complement to experimental studies. In this regard, we have developed an in-house set of tools to extract information from the AIMD simulations (*7*). The simulations will be performed using the VASP package (*8*).

The simulations (that will run on the national supercomputing centers) will focus on providing the density relations of these magmas, determining their chemical behaviour, and characterising their mechanical properties such as viscosity. We will try to relate the dissipation of the stresses with seismic attenuation. These results will provide a deeper understanding of the processes driving the formation and evolution of magmas in the shallow Earth and thus will better constrain the local dynamics of partial melting ascent.

Seismic wave propagation We use DSM Kernel Suite (*9*, *10*) that computes synthetic wavefield. DSM has been the most efficient and accurate synthetic seismogram computation method for 1D Earth models up to 2 Hz and DSM Kernel Suite proposes to use Born approximation (and Born series) to compute for 3D structure, together with DSM-Specfem injection method (*11*). During the master internship of L. Delaroque, we are updating the user interface of DSM Kernel Suite in order to facilitate and accelerate 1D/3D seismic wavefield computation for regional model perturbation.

Calendar The PhD project will involve conducting seismology and *ab initio* modelling in equal proportions concurrently.

Risk management Every main result in this project (*e.g.* physical properties of the magmas, DSM Kernel Suite software, seismic filtering, etc.) is publishable.

Collaboration This project brings together two different teams of IPGP (Seismology and CAGE), working on complementary methods. Moreover, it will use first-hand information provided by the Volcanological Observatory of Piton de la Fournaise. Stéphanie Durand (ENS Lyon) will participate for community code building.

Potential candidate: Lorraine Delaroque (M2 Université Grenoble Alpes) is currently working with N. Fuji on the development of next-generation code of DSM Kernel Suite for 3D waveform seismic filtering. Her strong skills in numerical modelling and coding as well as her solid background in seismology and physics, are ideal for pursuing this interdisciplinary project.

References

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