# PHD proposal :

### Numerical modeling of segregation and differentiation in partially melting orogenic crust

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 Co-supervisors : Thomas Bonometti (IMFT), Olivier Vanderahaeghe, Stéphanie Duchêne (GET)
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 Employer : CNRS MITI, French government (IRN FalCol). Starting october 2021.
 Location : GET OMP 14 avenue Edouard Belin, Toulouse, France.

**Terms of employment**: Contract aiming to obtain a PhD degree, with salary 2135 euros/monthn prior taxes for a period of three years in accordance with the agreement with CNRS MITI and SDU2E doctoral school.

## Application dead-line: july 25<sup>th</sup>, 2022. Audition interview (zoom) from july 20-28<sup>th</sup>, 2022.

**Application requirements :** The application should include a CV, documentation of educational merits, qualifications and previous activities. Skills in computational programming and in (petrology) thermodynamics are most required. A letter detailing personal motivations is welcome. If you have completed a degree abroad, it will be assessed by the doctoral school SDU2E before employment can take place.

**Project summary:** The aim is to develop a numerical coupling approach of thermodynamic and thermomechanical tools involved in the genesis of a partially melting crust and liquid/solid segregation, to bridge the gap between our understanding of the mineral scale metamorphic reactions and the crustal scale gravitationally driven viscous flow in response to external forces. This project aims at pursuing the development of OpenFOAM VOF solvers that were shown to track well crustal scale flowing heterogeneity interfaces (Louis-Napoleon et al., 2020, 2021). The incorporation of thermal and compositional interactions between distinct fluid phases will allow to investigate how these fluid phases evolve, migrate, and contribute to the entire crustal segregation balance.

Aim and objectives : Crustal differentiation is controlled by partial melting and magma fluid transfers. The circulation of such fluids has a decisive impact on the transfer of elements of economic interest (Chi & Xue, 2011). Understanding these processes is therefore essential to guide exploration and exploitation of subsoil resources. While the conditions for partial melting and crystallization are generally determined from thermodynamic modeling (Holland & Powell, 2011), the dynamic behavior of partially melting crusts is also approached by thermo-mechanical modeling (Poh et al., 2020; Piccolo et al., 2021; Schmeling et al., 2021). Some models take into account fluid-generating metamorphic reactions at the large scale, while others target segregation processes at the grain scale (eg. Petrella et al., 2021): our objective here is to link these scales with the support of field observation and laboratory petrology measurements. While research communities argue about the flow modes of magmatic fluids (eg. migration, mixing or reactive transport) and whether melt columns are chemically open systems at distinct depths (eg. Cornet et al., 2022), here we will seek to further formalize such processes at the intermediate scale.

Our primary field target is the **Eburnean belt of West Africa**, which testifies of a major crustal growth event around 2 Ga, and is composed of volcano-sedimentary series affected by greenschist metamorphism, granulites and intruded plutons. This belt is characterized by 10-30 km wavelength alternations between greenstone belts, and a dominant role of gravitational instabilities upon horizontal tectonics is debated (Ganne et al., 2014). The WAXI program (*waxi4.org/waxi-4/waxi-1-3/*) has gathered a unique database that highlights the role of the metamorphism of the volcano-sedimentary series in the genesis of migmatitic gneisses, fluids and their associated mineral resources (Masurel et al., 2021). Other targets will also serve as comparison: the Proterozoic Australian terranes, the Cretaceous European Alps and Naxos' migmatite domes (Siebenaller et al., 2013). Field and laboratory data will be used first to constrain the initial and limiting conditions of the models and guide the identification of major fluid transport modes (reaction, diffusion, localised, diapirism, convection), whereas the models in turn, will help seeking on the field, for the structural characteristics of « homogeneisation/segregation» processes. This inter-disciplinarity fosters in the context of the **IRN FalCol** french-australian network (*oceania.cnrs.fr/project/irn-falcol/*).

**Methodology** : The VOF numerical method is one of the best that conserve mass in multiphasic fluid flow, which becomes a major issue when understanding crustal segregation processes. The aim of this project is to pursue the development of solvers embedded in the opensource code **OpenFOAM** (*www.openfoam.com*) by incorporating the thermodynamic evolution of heterogeneous rock mass (e.g. adapt MagmaFOAM, Brogi et al.,2020; and Carrillo et

al., 2020). This control on compositions and rheologies of the matrix and liquids will help us identify the different scales of transport of fluid volumes (percolation via the porous medium or by convection-diapirism), and their impact on solid/liquid segregation. Particular attention will be dedicated to partial melting and crystallization reactions which play a role in the cycle of aqueous and carbonateous fluids participating in metallogenic processes (Petrella et al., 2021).

## Work plan

- \* Year 1 : hands on OpenFOAM starting at the crustal scale (setup as Louis-Napoleon et al., 2021) varying conditions and merging with thermodynamic conditions. Coding and publication 1 draft.
- \* Year 2 : Numerical implementation of a multiphysics solver for the 0.1-100 meters scale. Field work within the Falcol IRN network. 1 workshop/international conference.
- \* Year 3 : Results analysis, synthesis, and draft publication 2, conference. PhD ms. writing.

### Resources

\* Equipment : analytical platforms for petrological and geochronology analyses at GET (<u>www.get.omp.eu</u>), as well as the numerical equipment of the OMP community cluster Nuwa and the Olympe supercomputer from the CALMIP regional mesocenter (www.calmip.univ-toulouse.fr/).

\* Fieldwork, traveling, and conferences expenses will be supplied for by national grants and FalCol.

**The Lab:** GET (Geosciences Environnement Toulouse) is a multi-disciplinary research laboratory attached to the Midi-Pyrénées Observatory (OMP). It is a so-called mixed unit (CNRS, IRD, P. Sabatier University, CNES) that brings together about 226 people. Research themes include studies of the internal Earth, its surfaces and continental interfaces, to improve knowledge on (i) the evolution and dynamics of the Earth, (ii) spatial and in situ observation of the Earth, (iii) the critical zone and fluid-rock-living interactions, and (iv) geo-resources and Contaminants-Environment-Health interactions. This PhD will be part of the TIL team (Terre Interne Lithosphere, *www.get.omp.eu/til/*), which studies the dynamics of the Inner Earth from a petro-structural point of view.

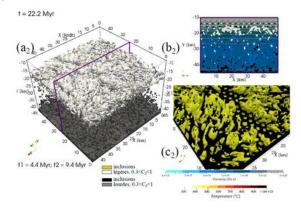
This PhD will be co-supervised by academic researchers:

i) Muriel Gerbault (<u>www.get.omp.eu/author/muriel-gerbault/</u>), IRD GET, applies solid and fluid mechanics numerical methods to a variety of geodynamic and volcano-tectonic deformation contexts.

ii) Nicolas Thébaud (<u>www.research-repository.uwa.edu.au/en/persons/nicolas-thebaud</u>), UWA, is a geologist specialised in the metallogenic (and metamorphic) provinces of Australia and Africa, and

iii) Thomas Bonometti (<u>www.imft.fr/pages-personnelles/bonometti-thomas/</u>) is a fluid mechanics VOF method expert at IMFT (Institute of Fluid Mechanics, Toulouse), which hosts several OpenFoam experts.

Figure: 3D simulation with OpenFOAM for the formation of metamorphic domes in a heterogeneous, convecting, partially melting continental crust (light white inclusions convect and stack below the upper crust). After Louis-Napoléon (2020).



#### Some references

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Petrella, L., Thébaud, N., et al. (2021). Competitive fluid-rock interaction processes Geochim. Cosmochim. Acta, 313, 38-54.
Piccolo, A., Kaus, B. et al. (2020). Plume-Lid interactions during the Archean. Gondwana Research, 88, 150-168.
Poh, J., Yamato, P., et al. (2021). Transition from ancient to modern-style tectonics. Gondwana Res. 99, 77-92.
Siebenaller, L., Boiron, M., et al. (2013). Fluid record of rock exhumation (Naxos Island). J. Metam.Geol. 31(3), 313-338.