Université de Paris

Labex UnivEarthS

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IPGP Frontier Project

The creation and preservation of chemical heterogeneities in Earth's primordial magma ocean

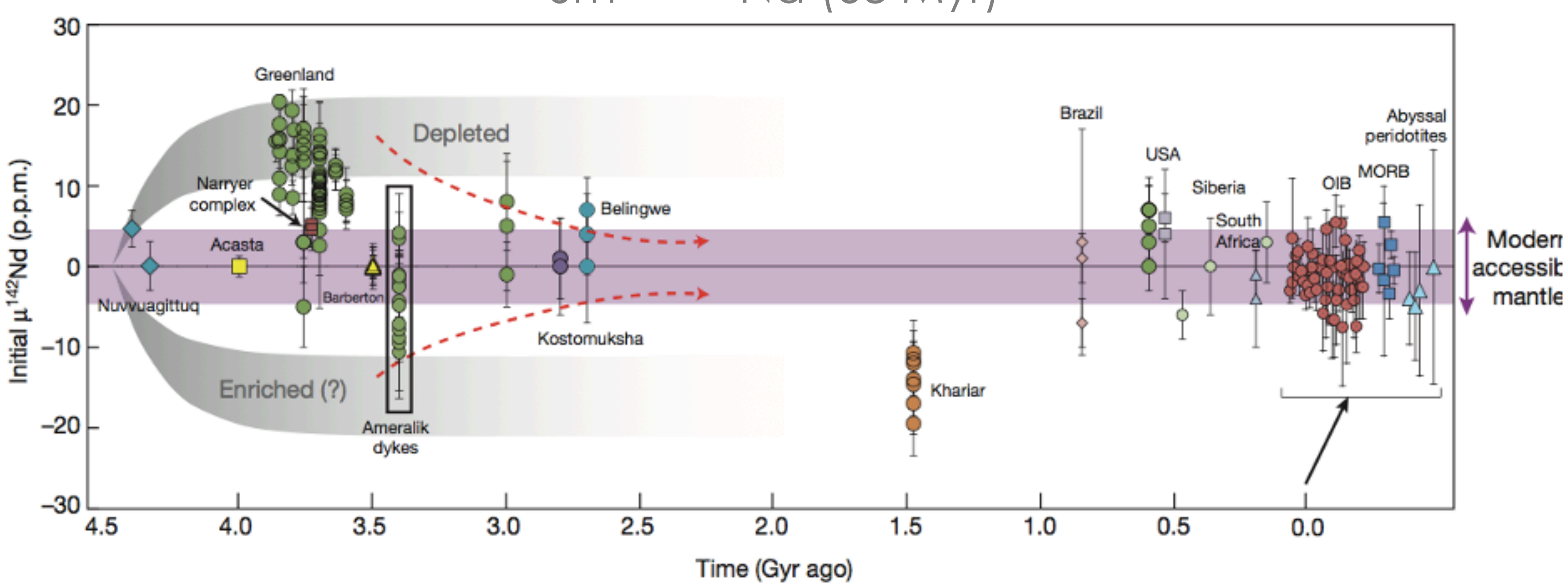
Leader: James Badro

Co-leaders: Maylis Landeau and Henri Samuel

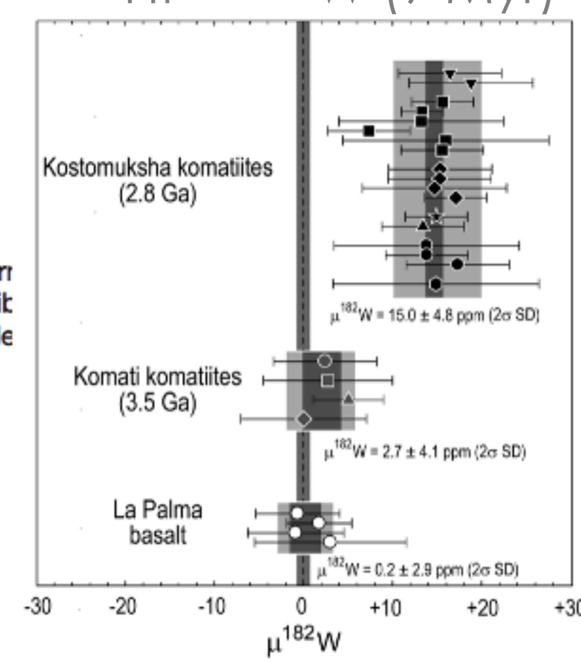
+ Charles-Édouard Boukaré, PhD student

The Setting

$^{146}Sm \rightarrow {}^{142}Nd$ (68 Myr)

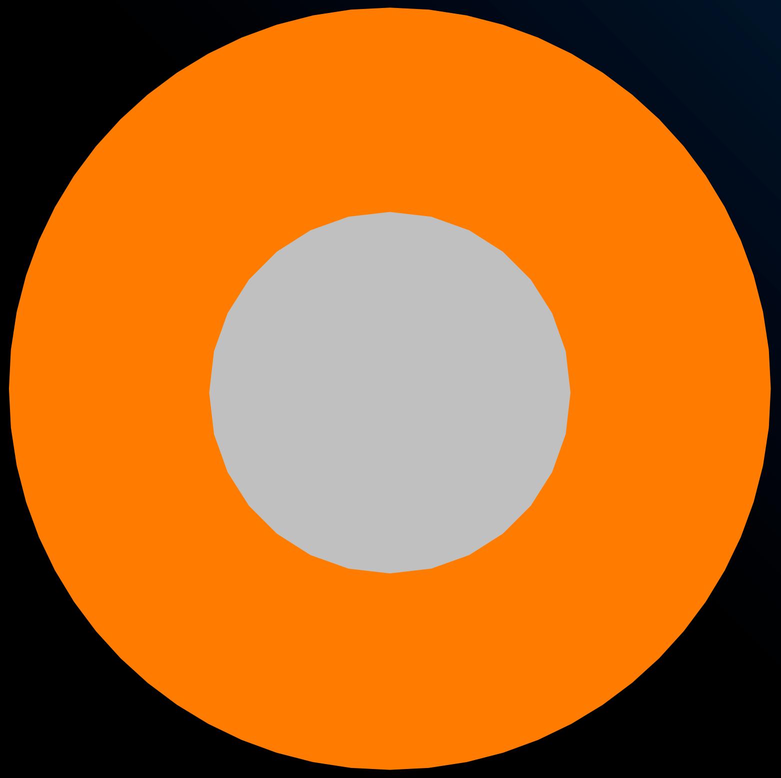


$^{182}Hf \rightarrow {}^{182}W$ (9 Myr)



The Setting

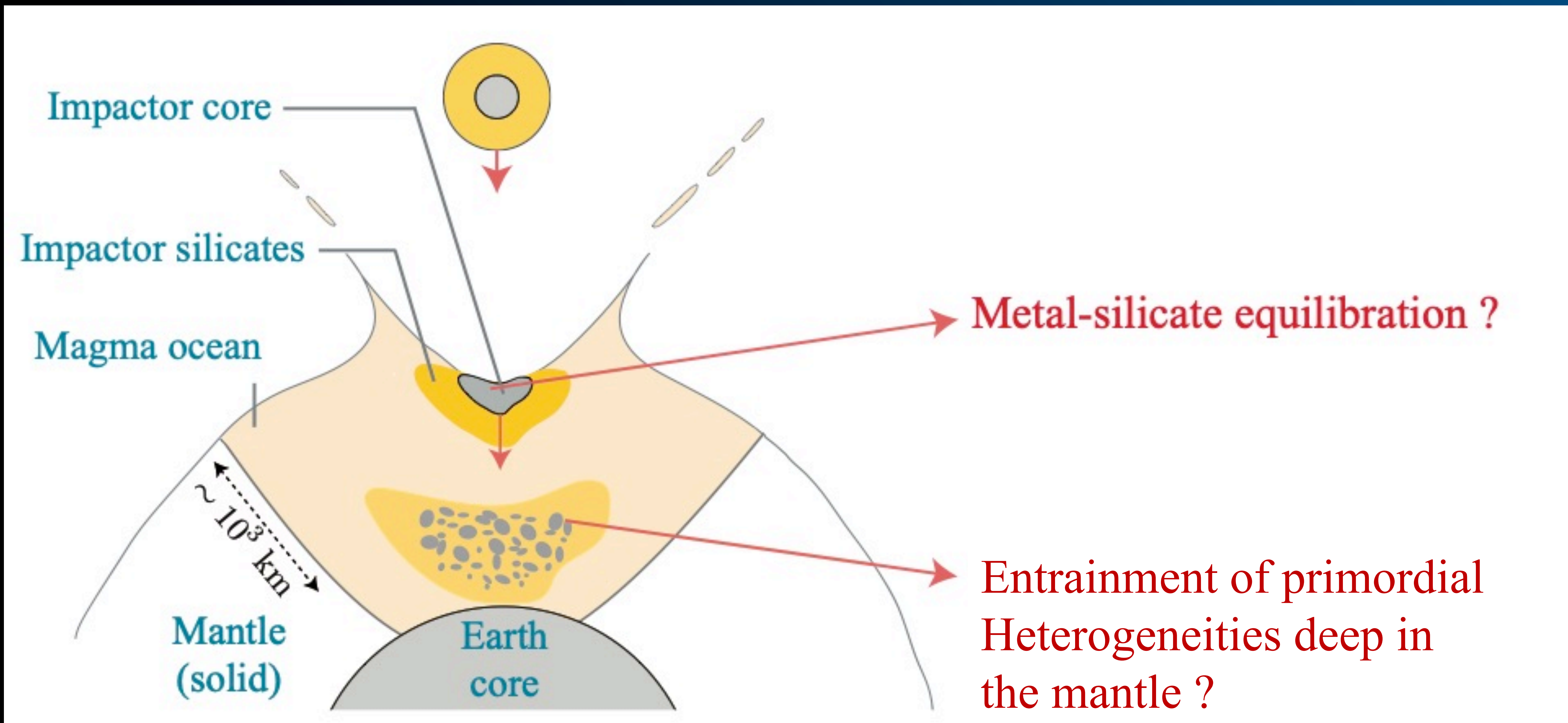
Earth before crystallisation
Fully molten planet



Earth during crystallisation
Solidification of the planet

Earth after crystallisation
Initial conditions (composition and spatial distribution of mantle heterogeneities)

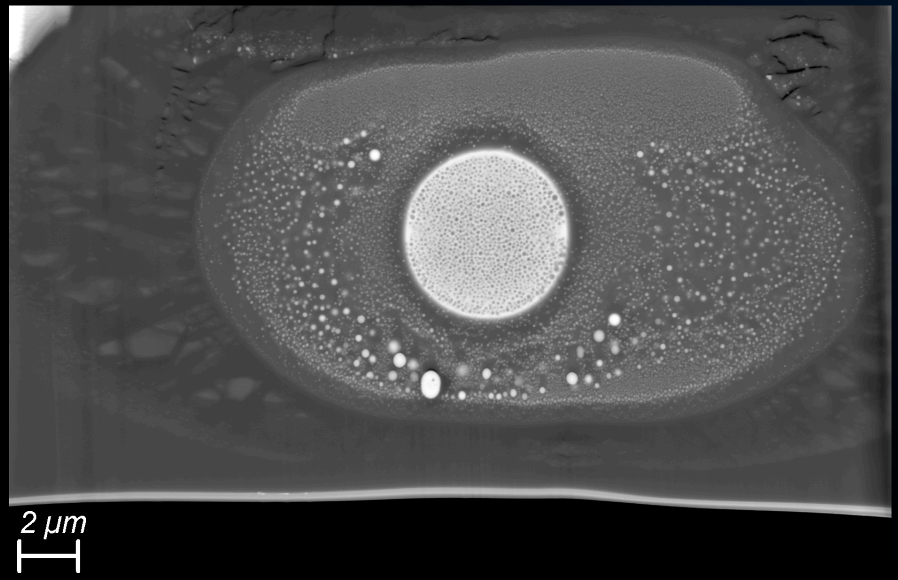
Task 1: Chemical heterogeneities during accretion (impacts)



Task 1: Chemical heterogeneities during accretion (impacts)

High P-T experiments

Metal-silicate phase equilibria

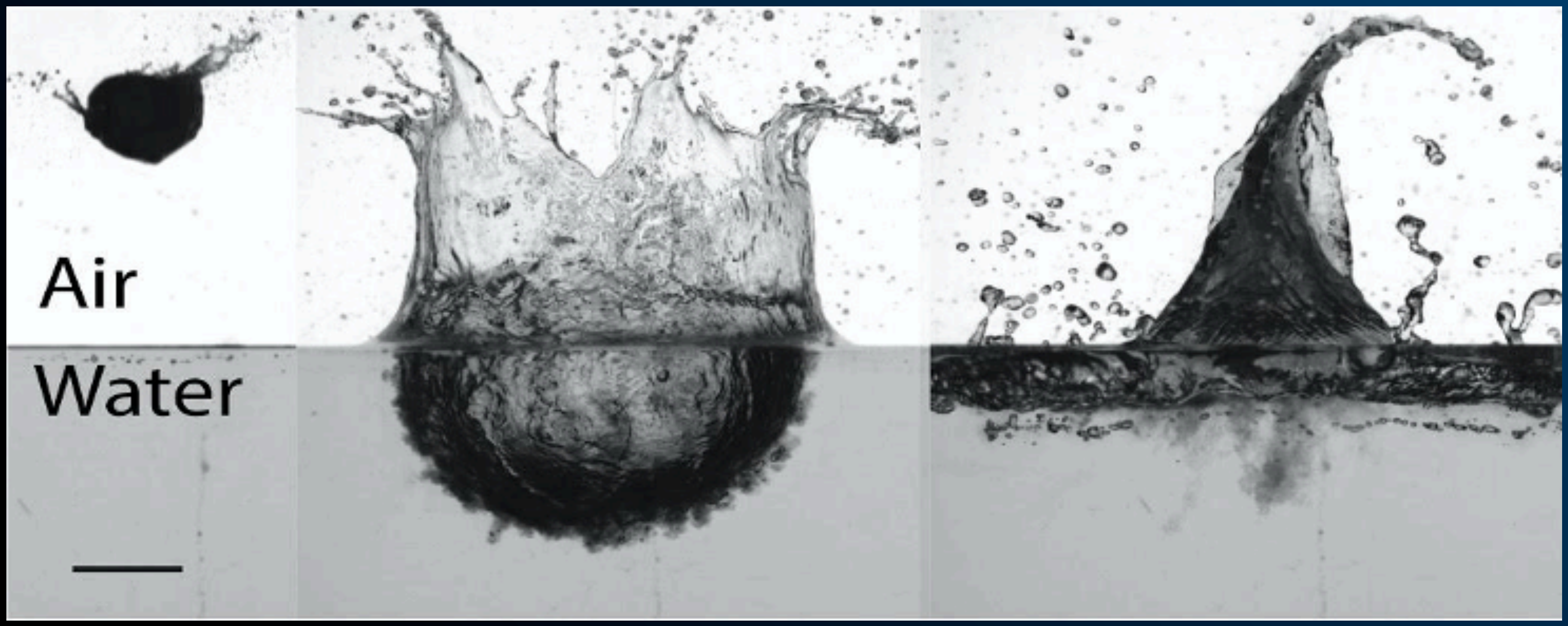


Chemical heterogeneities in the magma ocean

Impact experiments

Can heterogeneities be destroyed by impacts, entrainment and remixing ?

Two-phase fluid dynamics experiments and high-speed imaging



Task 1: Chemical heterogeneities during accretion (impacts)

- The experimental setup is operational at IPGP (M. Landeau) and has been used to understand metal-silicate (i.e. core-mantle) entrainment and mixing

- Need to adapt the experimental setup to look at how silicate melts with different composition and buoyancy get entrained and remixed

- This can be done with small mods on the setup (small equipment) and adapting the imaging software

- This will be done with a PhD student (funded by doctoral school)

- Should obtain scaling laws that allow us to infer the type of heterogenies that can be preserved, and the bounds on their composition in order to maintain them

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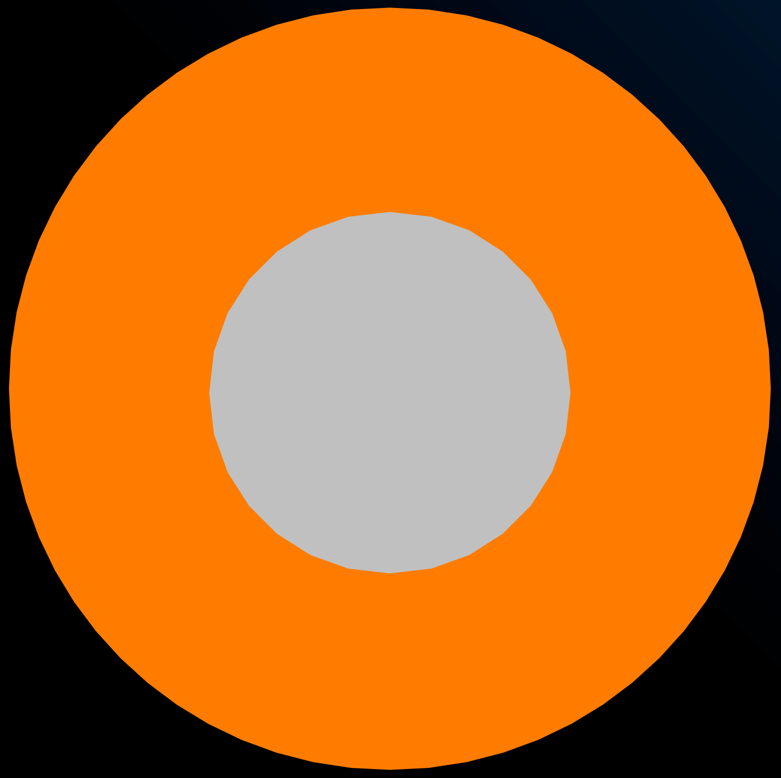

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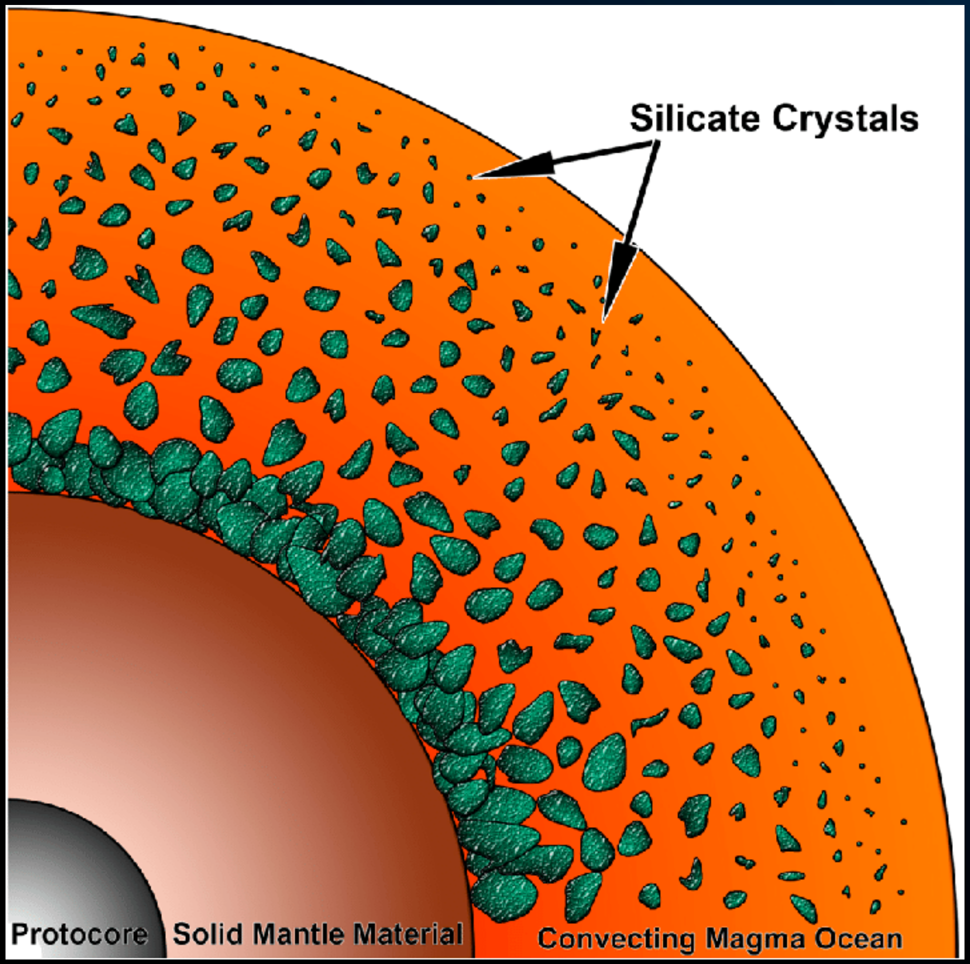
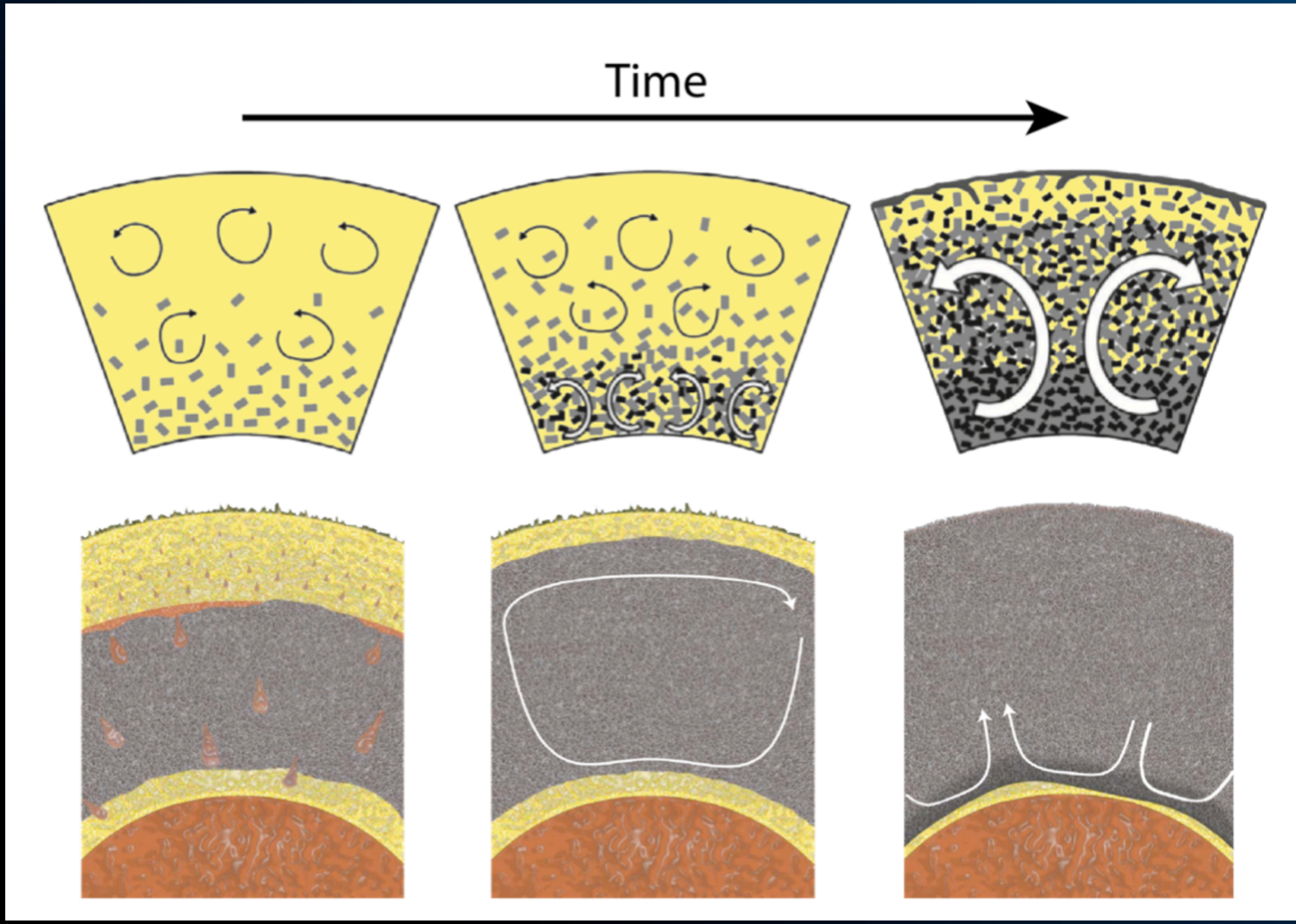
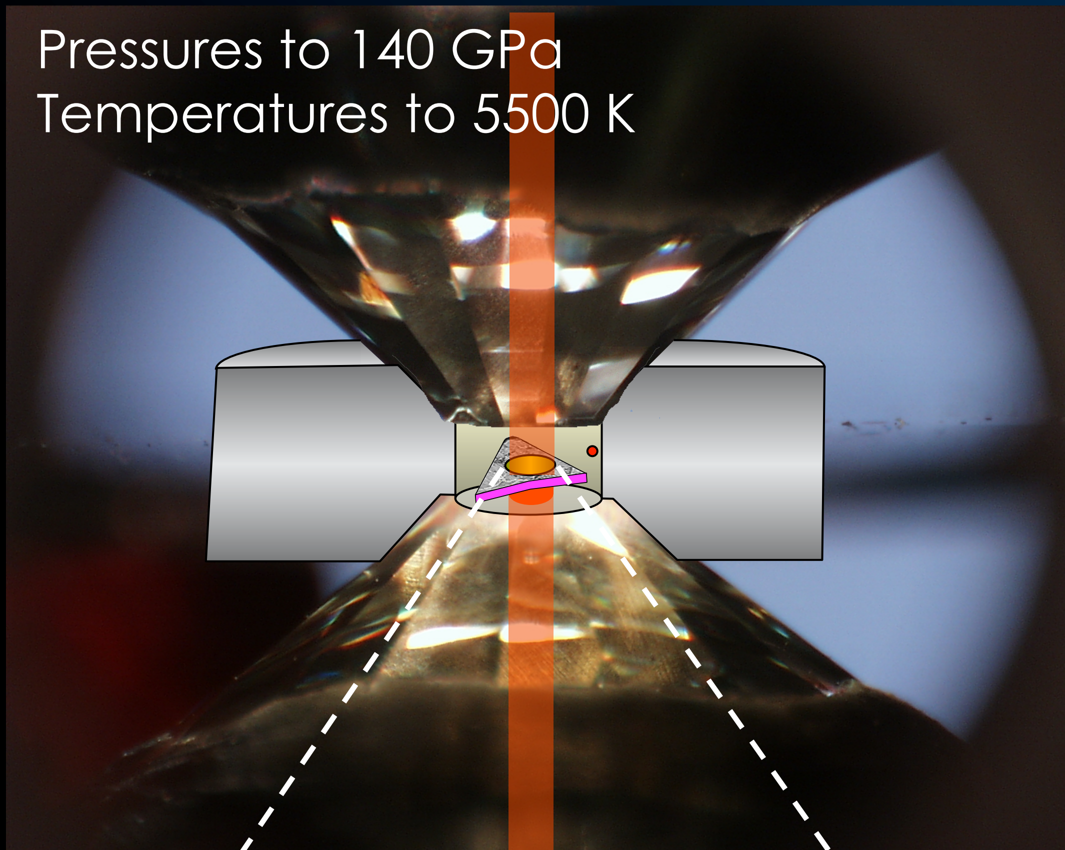
Earth after crystallisation
Initial conditions (composition and spatial distribution of mantle heterogeneities)

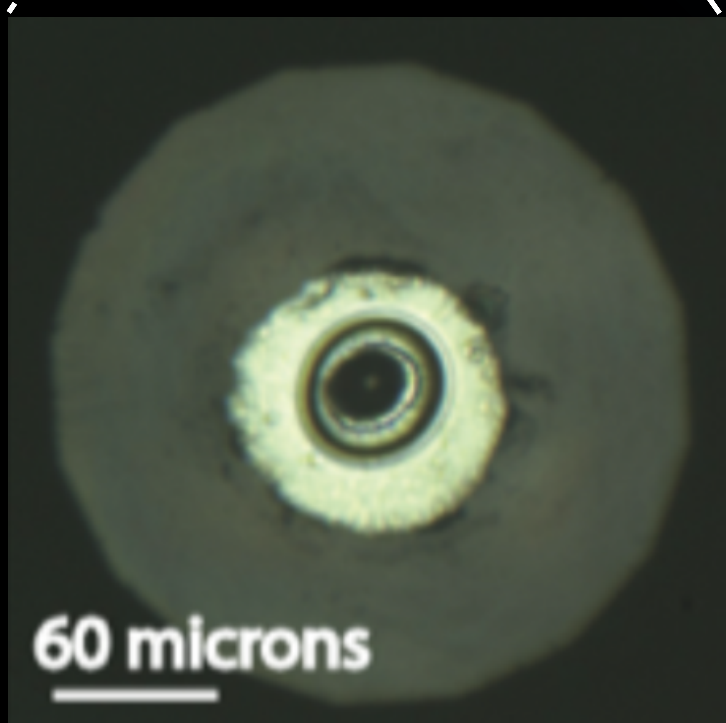
Task 2: Chemical heterogeneities during mantle solidification



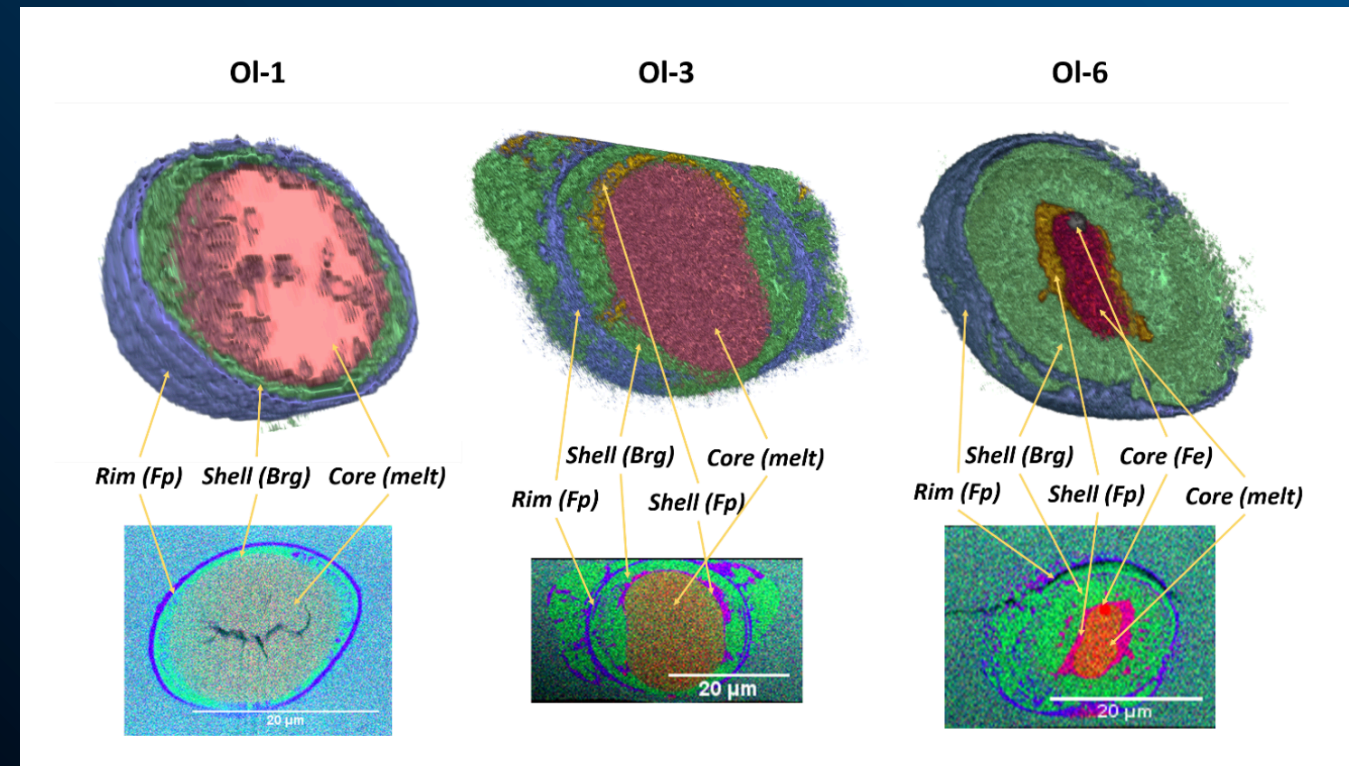


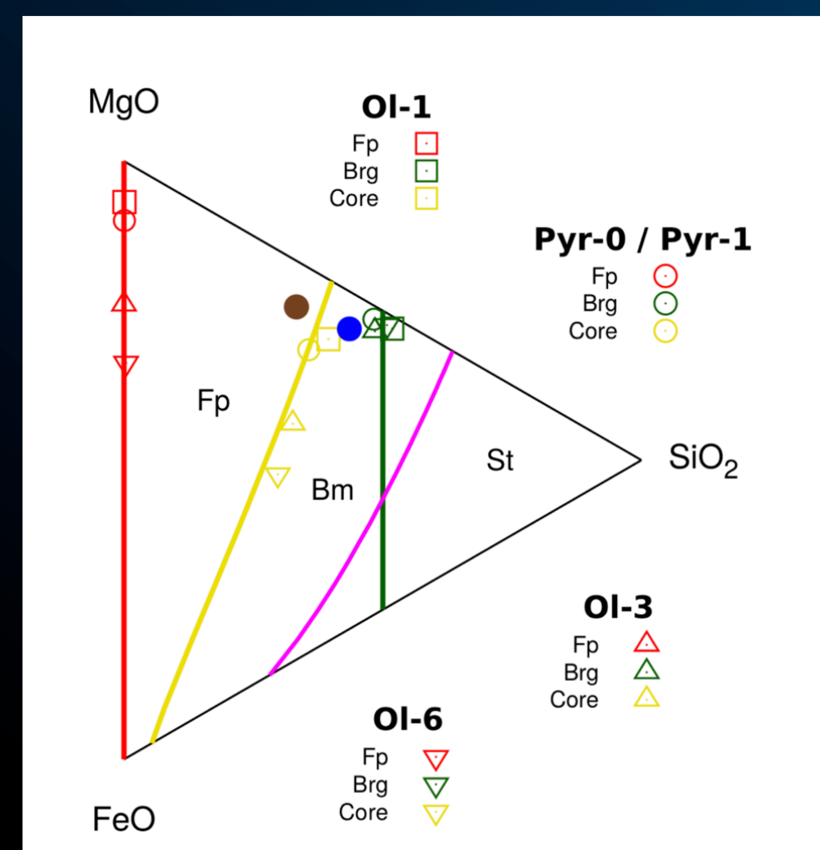
Task 2: Phase equilibria and melting relations in the deep mantle





52 GPa 3300K–3000 K





Task 2: Phase equilibria and melting relations in the deep mantle

- The experimental setup is operational at IPGP (J. Badro) and has been used to understand metal-silicate (i.e. core-mantle) chemical interactions
- We have shown that we can also use it to study the crystallisation of silicates at deep mantle conditions
- Need to carry out more experiments using the protocol we have put forth, at various pressures (3 more between 70 and 135 GPa)
- This can be done straight away, and requires funds to carry out the analyses. Each pressure point requires ~6 experiments, and each one requires 2 days of FIB and 1 day of TEM (3 k€)
- This will be done by J. Badro, possibly with a PhD student currently in M2 (funded by doctoral school)
- Should obtain melting relations and phase diagrams for the mantle at all depths, and allow us to describe how the mantle crystallises (which phases, what composition, what buoyancy contrast) at any depth

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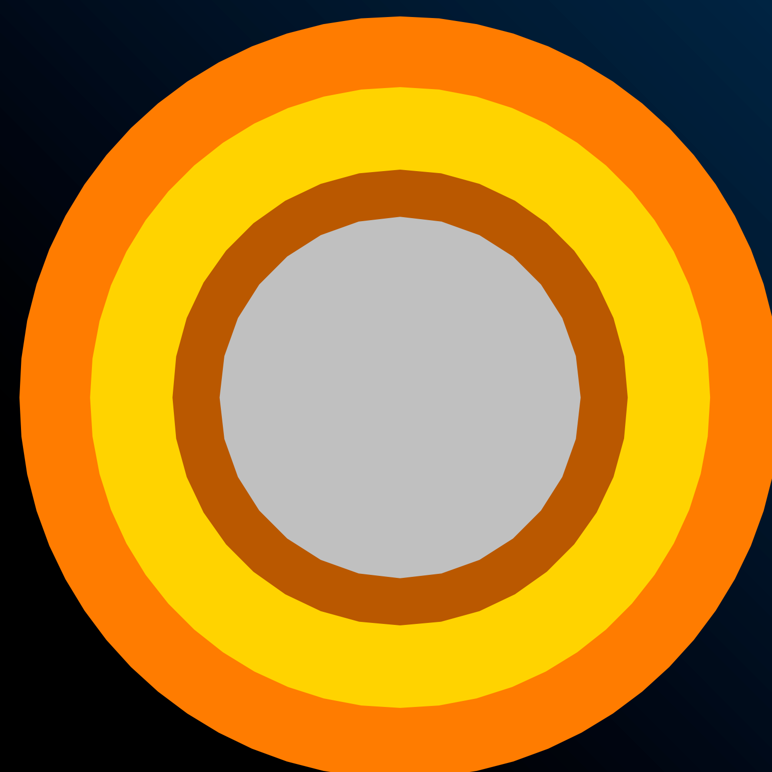
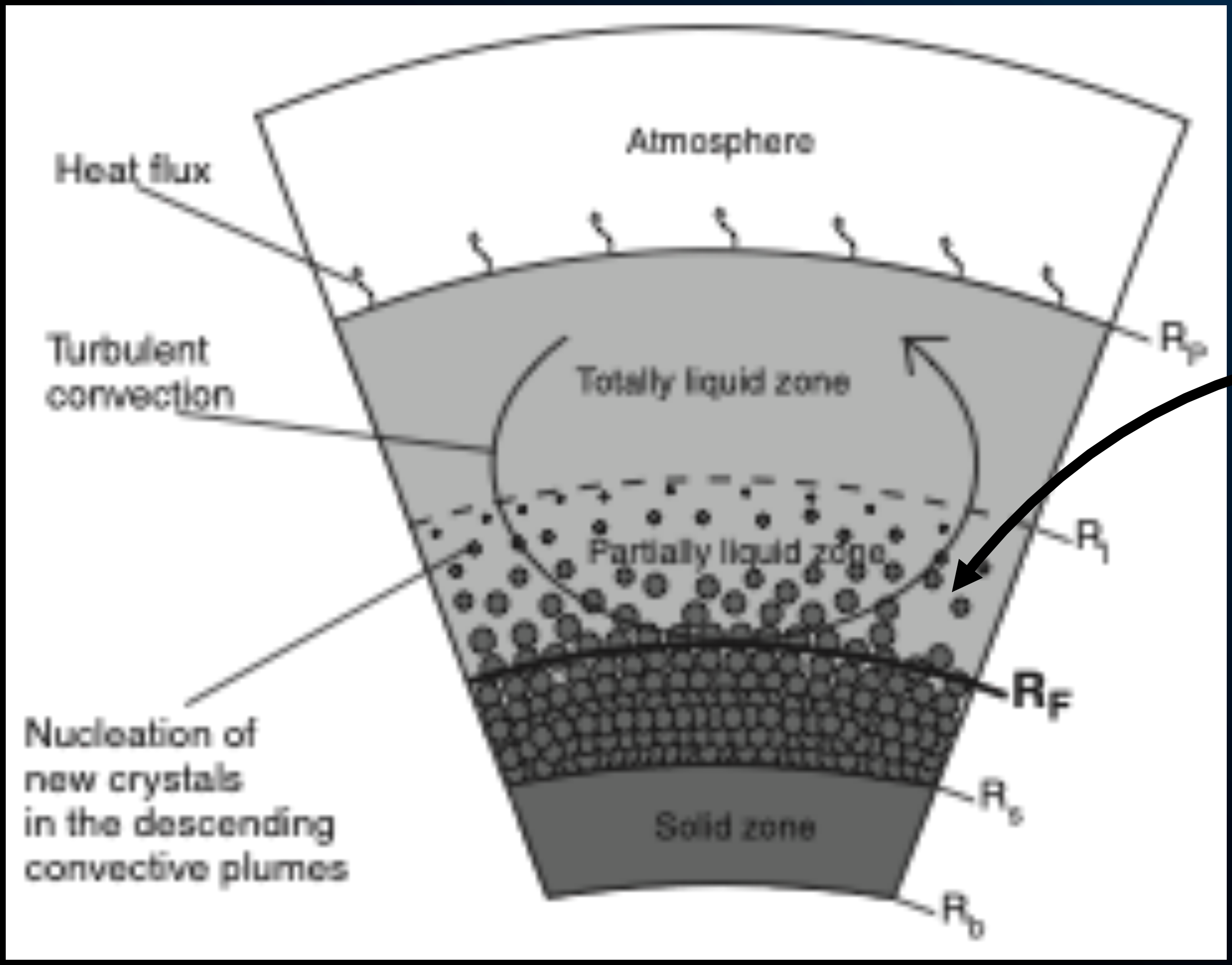
Solidification of the planet



Earth after crystallisation
Initial conditions (composition and spatial distribution of mantle heterogeneities)

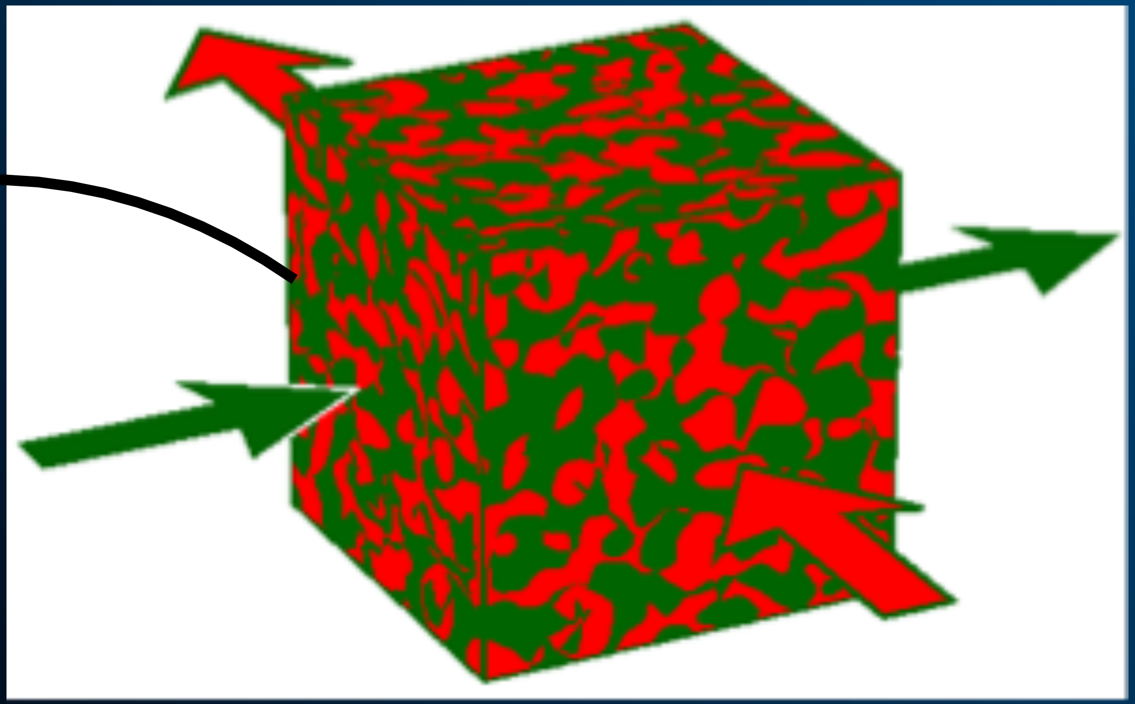
Task 3: Differentiation of a convecting and crystallising magma ocean

Crystallising terrestrial silicate magma ocean



[Solomatov, 2004; Lebrun al., 2013]

Two-phase flow averaged equations



[Bercovici et al., 2001]

Cooling & solidification: coexistence of liquid fraction (ϕ) and solid fraction (1-ϕ) phases

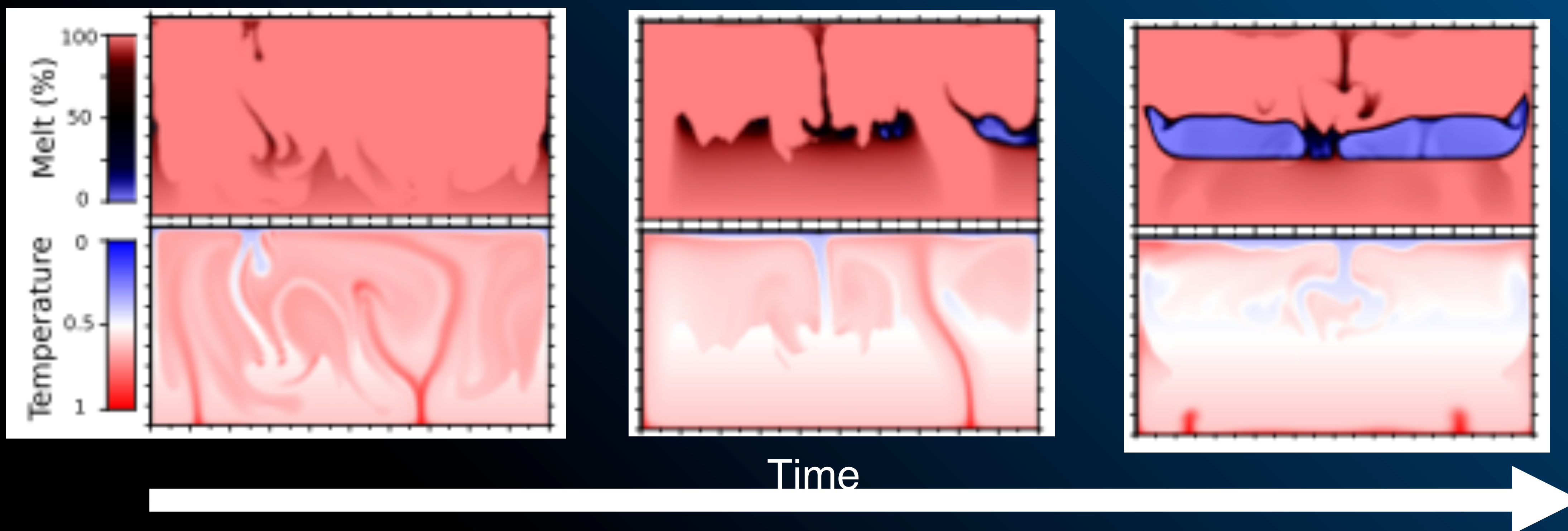
✔ Interacting liquid/solid fractions decrease or increase locally

✔ Chemical differentiation via element solid-liquid partitioning

✔ Variety of non-linear melt/solid interactions (segregation, compaction, remelting, etc.)

Task 3: Differentiation of a convecting and crystallising magma ocean

Modelling tool: *Boukaré & Ricard [2017]'s* finite difference code to solve the two-phase flow averaged equations (conservation of mass, momentum, energy, phase separation, and phase transport)



[Boukaré & Ricard, 2017]

Advantages

- Can model the solidification of a convecting two-phase mixture for all crystal fractions
- Accounts for melt fusion and crystallisation, including latent heat/cooling effects

Current limitations

- Cannot handle realistic (large) solid-melt viscosity contrasts or (P,T) variations
- Advective transport prone to significant amounts of numerical diffusion
- Sequential code
- Direct matrix inversion scheme computationally prohibitive

➪ Limited to coarse grid resolution and unrealistically small Rayleigh numbers

Task 3: Code enhancement & tuning + exploration of the governing parameter space

Task 3: Differentiation of a convecting and crystallising magma ocean

- The two-phase numerical convection code exists and was written by Charles-Édouard Boukaré and has been used to understand the evolution of a crystallising silicate mantle

- It can handle the parsing of phase relations that will have been determined in WP2

- The code needs however to be adapted and optimised

    - Adapted to handle large viscosity contrasts by including methods developed by Henri Samuel

    - Optimised by using efficient solvers and parallelized to run on (and take profit of) the GENSI HPC ressources

- Should obtain the dynamical evolution of a crystallising magma ocean, with the built-in thermodynamic consistency of experiments. This should give us a dynamical picture of what sorts of produced heterogeneities can be maintained, where in the mantle they would reside, and what is the intial state of the solid mantle with repsect to primitive heterogeneities and the distribution of heat-producing elements

The Team

Chemical evolution of the mantle from the ***early*** molten state to the ***modern*** solid state

Bring together an age and gender balanced team of leaders in their fields in:

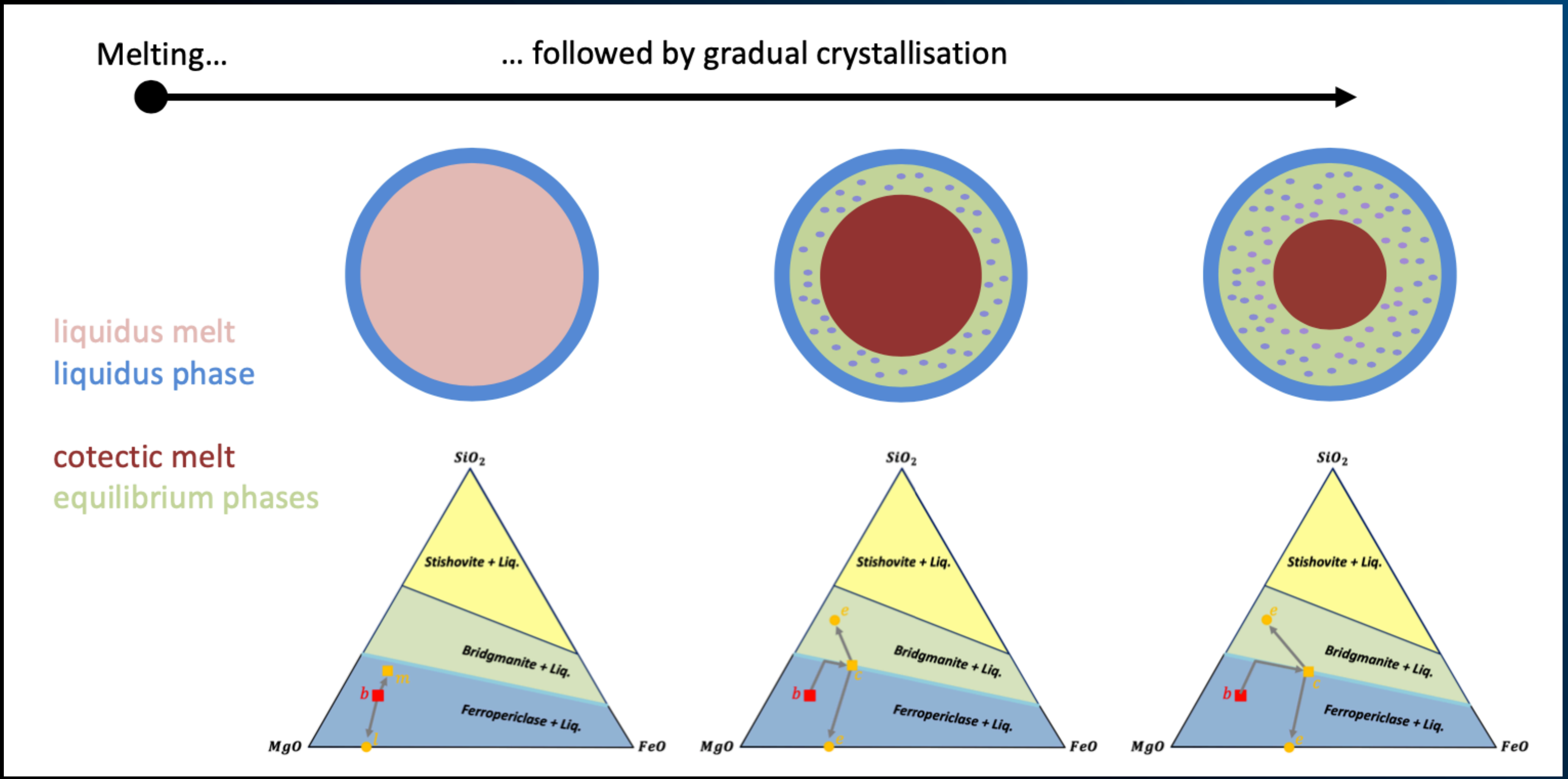
- Experimental fluid dynamics
- Experimental petrology
- Thermodynamical Modelling
- Numerical geodynamics

Benefit from the extraordinary potential we have at UP/IPGP to carry out this proposal

Workplan

ITEM DESCRIPTION	WORKPACKAGE	BUDGET	DESCRIPTION
PhD student	**WP1**	**0**	**Funded by UP/IPGP doctoral school**
Postdoc (ChEd Boukaré)	**WP3**	**110 000**	**Develop the convection code (with Samuel) based on the Boukaré 2015 & 2017 framework, and incorporate the thermodynamical data (with Badro) obtained in WP2.**
Consumable cost	**WP1**	**5 000**	**These are consumables for WP1. Badro has enough own-funds to cover the consumables of WP2. No consumables for WP3.**
Analytical cost	**WP2**	**55 000**	**FIB and TEM analyses.**
Mission cost	**All WPs**	**20 000**	**Conferences** **Analyses at EPFL (Switzerland)**
Equipment costs	WP1, WP3	14 000	Laser for WP1 (5 k€) Workstation for WP3 (11 k€)

Task 2: Phase equilibria and melting relations in the deep mantle



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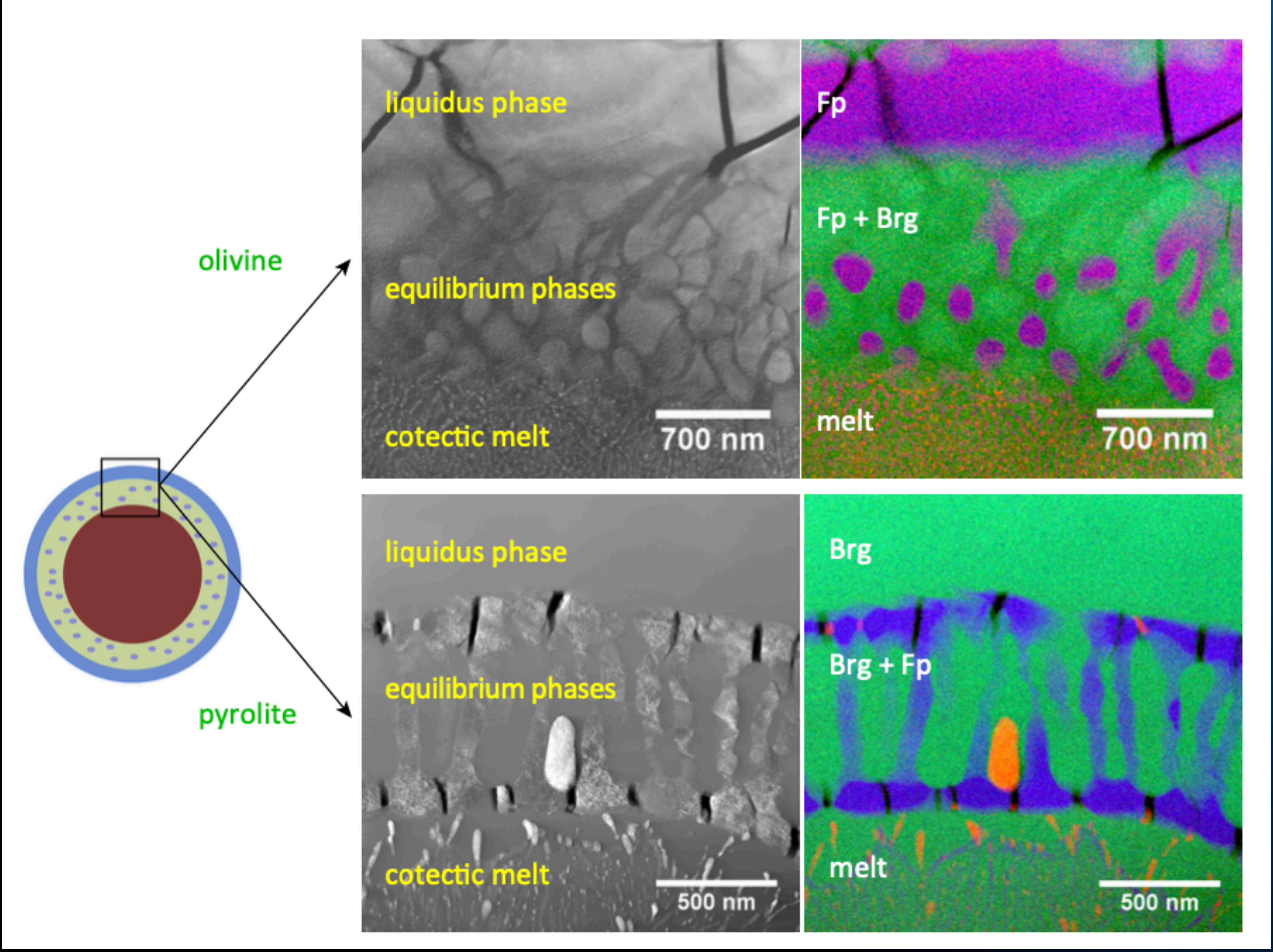
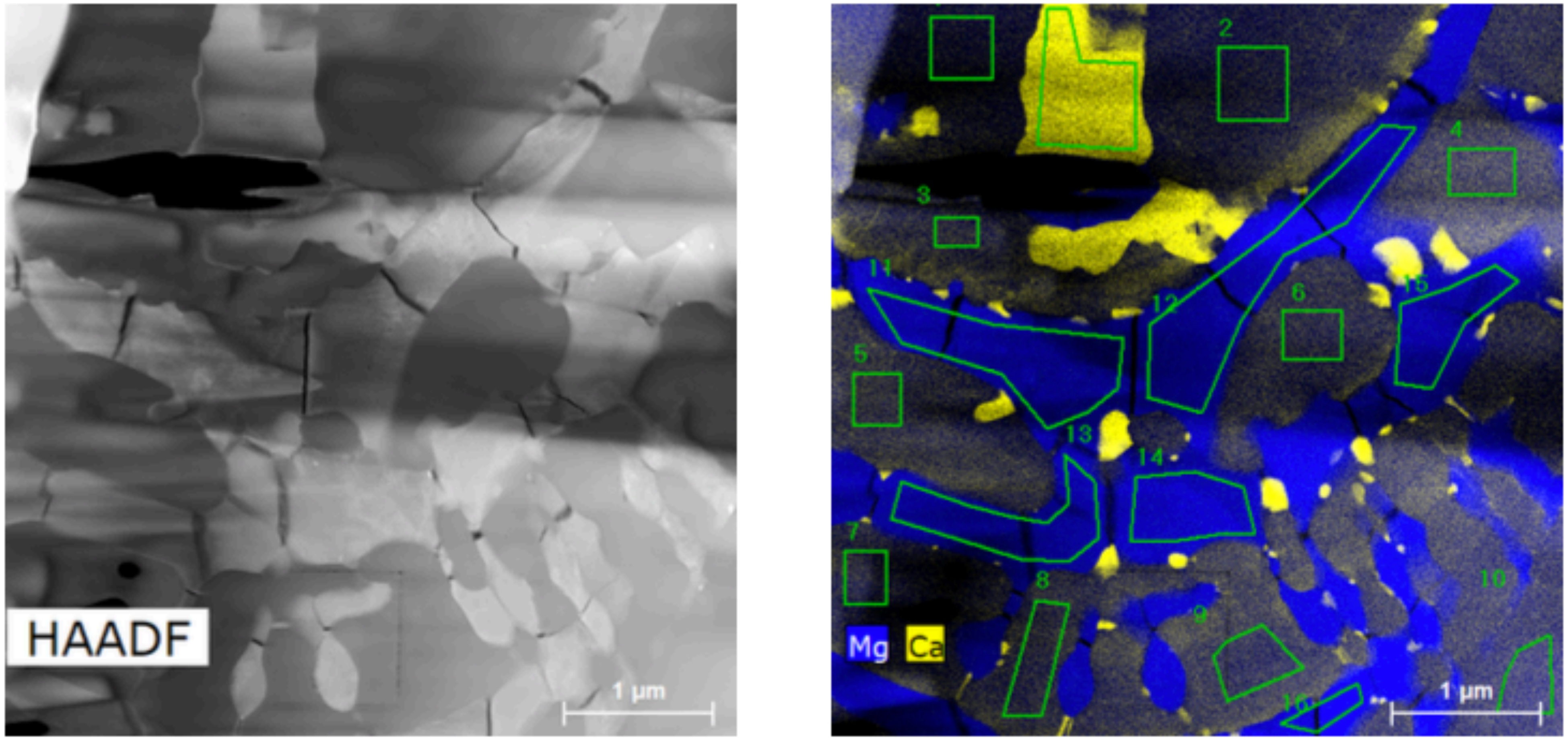


Task 2: Phase equilibria and melting relations in the deep mantle

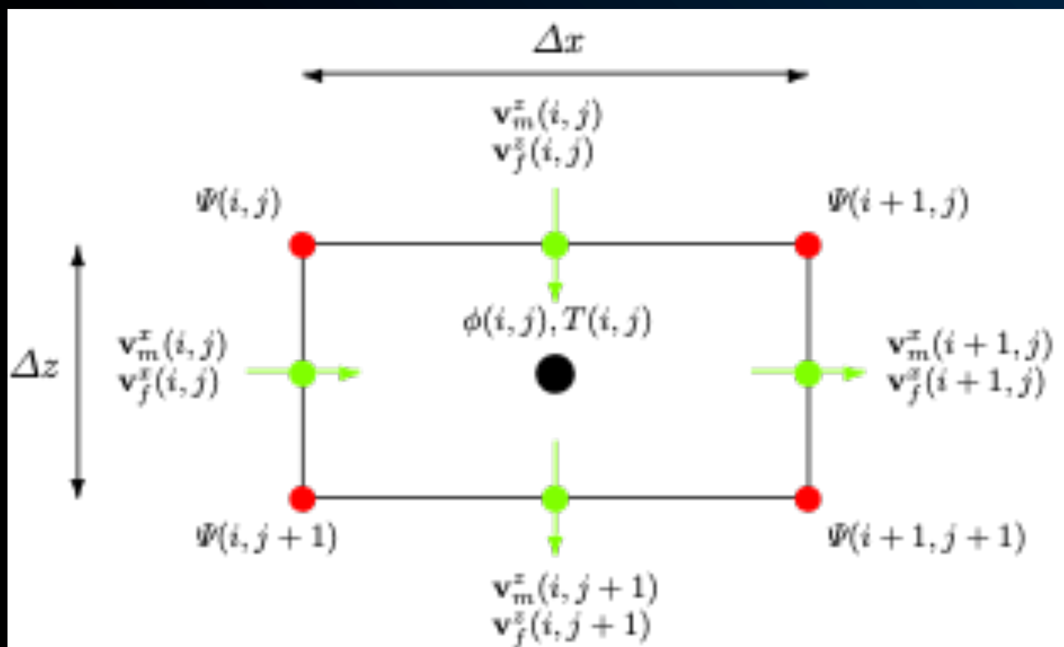


Brg	NdO1.5	SmO1.5	LuO1.5	UO2
conc (ppm)	1386	1993	1080	76
std err (ppm)	487	475	143	65

Task 3a: Including sharp viscosity contrasts in the numerical model

Conservation of total momentum: $$-\nabla\Pi + \nabla\cdot\left[\eta\left(\nabla\mathbf{u} + \nabla^T\mathbf{u}\right)\right] + Ra\, T\mathbf{e}_z + Ra\, B\, \phi\mathbf{e}_z = 0$$

Boukaré & Ricard [2017]'s code: streamfunction on a staggered grid

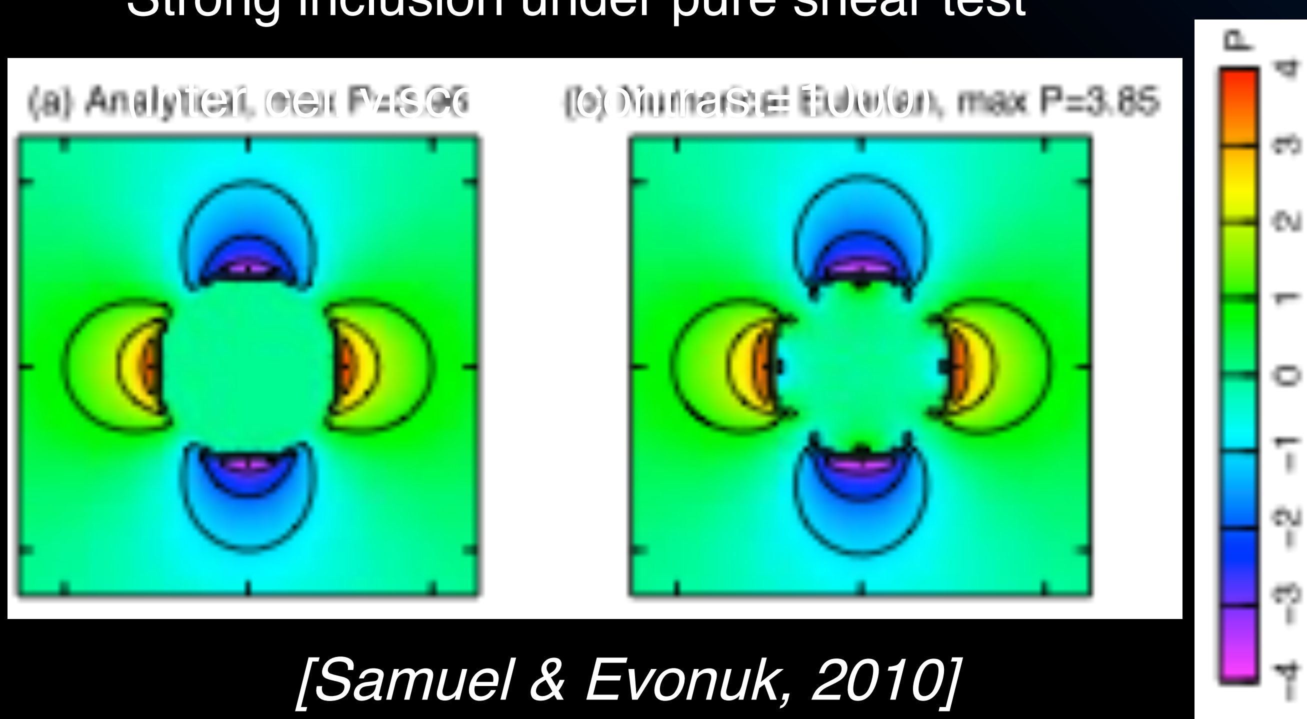


Problem *Viscosity ratio:* $\xi = \eta_s/\eta_l$

Sharp viscosity variations can cause spurious numerical instabilities with this formulation

➪ Solid-liquid viscosity contrasts could not be accounted for in *Boukaré & Ricard [2017] : ξ=1*

Strong inclusion under pure shear test



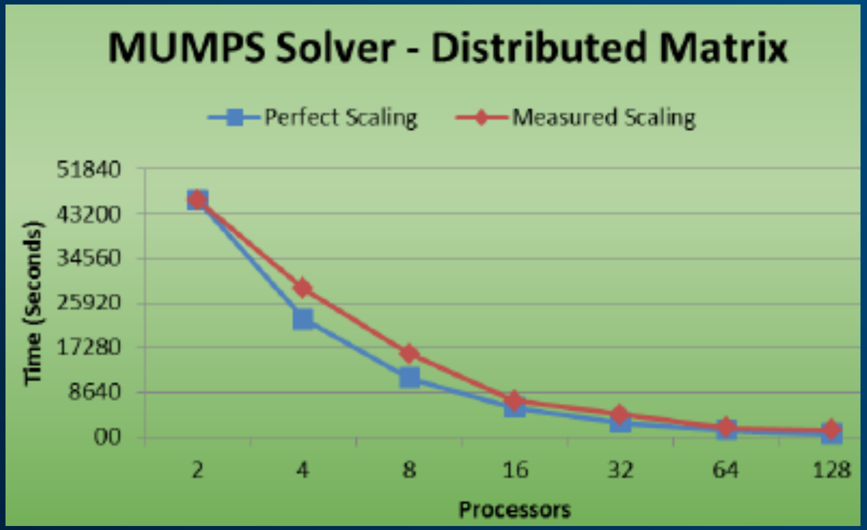
[Samuel & Evonuk, 2010]

Solution

Modification of *Boukaré & Ricard [2017]*'s finite-difference stencils following *Samuel & Evonuk [2010]* to handle significant viscosity variations : $\xi > 10^{10}$

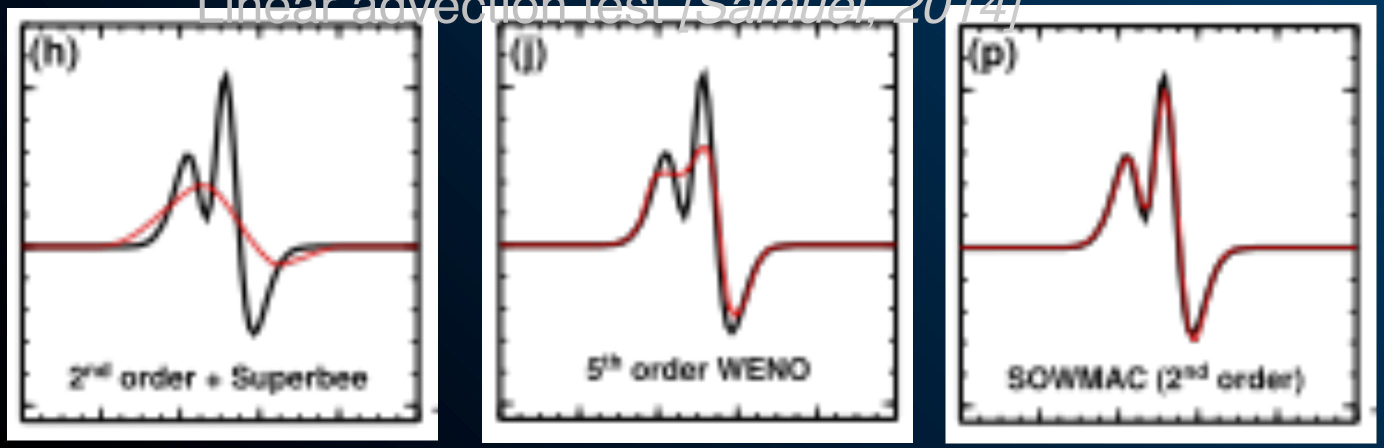
Task 3b: Increasing computational efficiency and accuracy of the numerical scheme

Code efficiency problem
Momentum & generalised Darcy equations currently solved via direct matrix inversion
➪ Computational time ~ Unknowns^3
➪ Limited to low resolution & small Rayleigh numbers



Code efficiency solution
Using efficient parallel direct sparse matrix /iterative solvers
➪ Multiple choice of solvers: MUMPS, PARDISO, superLU…
➪ Computational time ~ Unknowns - ~Unknowns^2
➪ Parallelisation
➪ Can reach relevant *Ra* for partially molten magma oceans

Linear advection test *[Samuel, 2014]*



True solution

Accuracy problem for transport equations
Current code uses an implicit scheme (ADI)
➪ Scheme prone to artificial diffusion
➪ Accuracy decreases with model time

Accuracy solution for transport equations
Replace ADI by efficient explicit schemes (*e.g.*, WEM-SOWMAC *[Samuel, 2014]*)
➪ Very small numerical diffusion despite being purely Eulerian
➪ Low order & nearly computationally optimal (negligible cost compared to momentum solve)

Task 3c: Including solid–melt partitioning in the geodynamic code

Need to implement trace element partitioning between the melt and solid phases

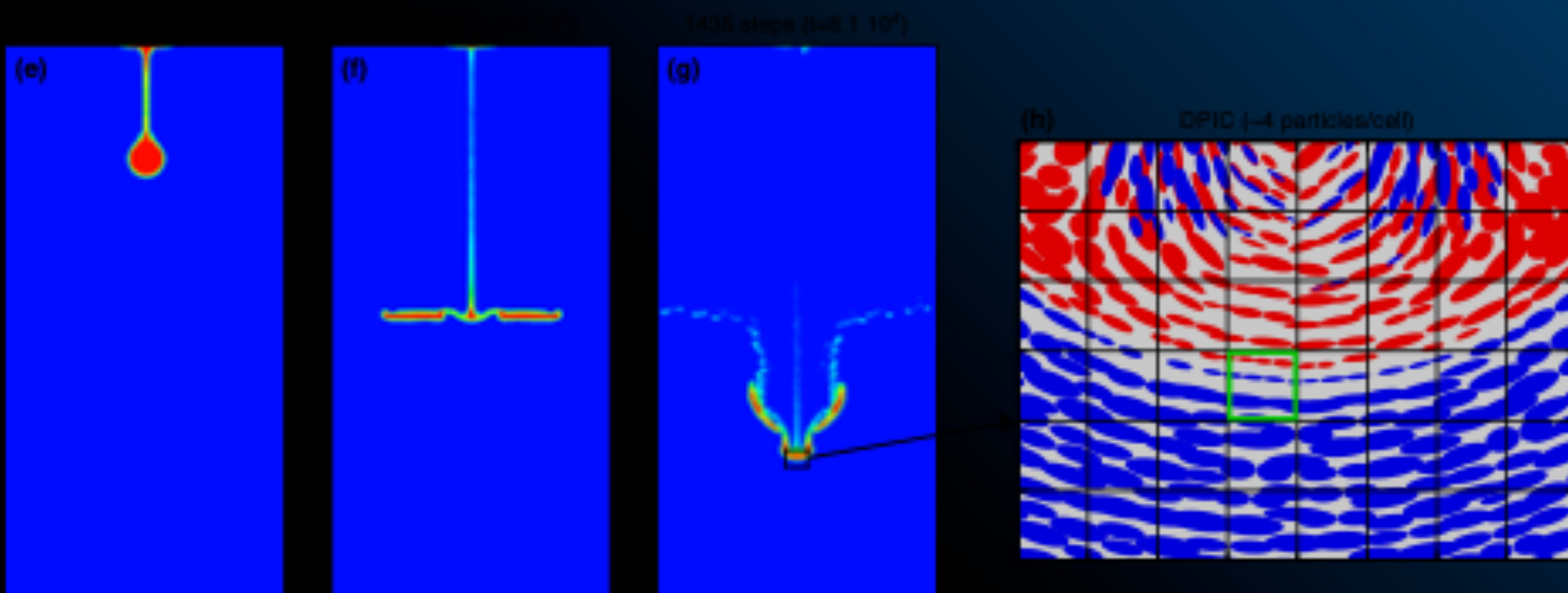
➪ Adopt a Eulerian-Lagrangian approach via particles

➪ Track the chronology of the crystallisation sequence until complete solidification

➪ Track the transport of active (*e.g.,* heat-producing elements) or passive species (Sm, Nd, Lu, Hf)

➪ Account for element partitioning upon melting or solidification using partition coefficients (**Task 2**)

➪ Negligible amount of numerical diffusion *[Samuel & Evonuk 2010; Samuel, 2018]*



Questions to address

✔ Under which conditions can the crystallization of the partially molten magma ocean result in a heterogeneous early solid mantle?

✔ What are the nature and the corresponding scales of heterogeneity resulting from the complete solidification of a terrestrial magma ocean?

✔ Can the freezing of a partially molten magma ocean result in some form of mantle layering that could remain preserved during the subsequent long-term evolution of the mantle?

Parameter space to be explored

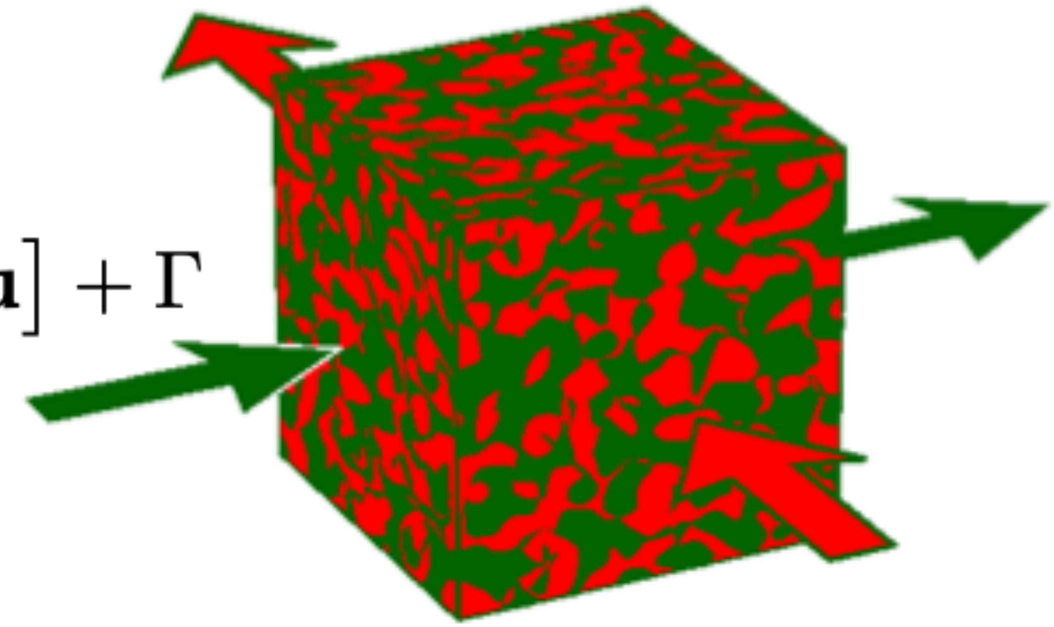
Rayleigh number	Buoyancy number	Permeability
		$\epsilon = k_0/L^2$
Convective vigour	*Compositional/phase vs. thermal density contrasts*	*Pore dimension*
Systematically varied	*Experimentally constrained **(Task 2)***	*Systematically varied*

+ various initial conditions using the results from impact mixing scenario experiments (**Task 1**)

Two-phase flow averaged equations *[Boukaré & Ricard, 2017]*

Conservation total momentum: $-\nabla\Pi + \nabla\cdot\tau + Ra\ T\mathbf{e}_z + Rb\ B\ \phi\mathbf{e}_z = 0$

[Bercovici et al., 2001]



Conservation of mass: $\nabla\cdot\mathbf{u} = 0$

Conservation of phases: $$\frac{D\phi}{Dt} = \nabla\cdot\left[\phi(1-\phi)\nabla^2\mathbf{u}\right] + \Gamma$$

Conservation of energy: $$\frac{DT}{Dt} = \nabla T + Q + \Gamma S_t$$

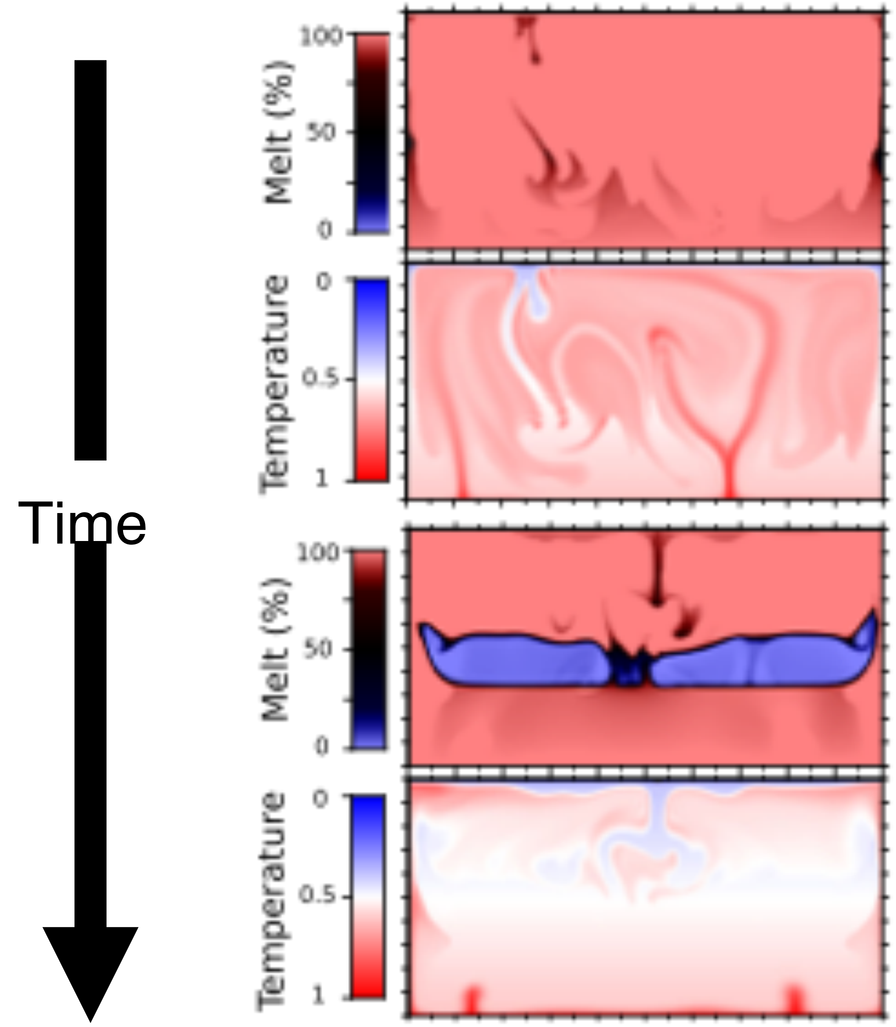
Phase separation: $$\phi\nabla^2\mathbf{u} = \epsilon\ \xi\phi^2\left[\nabla\cdot\tau + \nabla\left(\frac{1-\phi}{\phi}\nabla\cdot(\phi\nabla^2\mathbf{u})\right) + (1-\phi)Ra\ B\mathbf{e}_z\right]$$

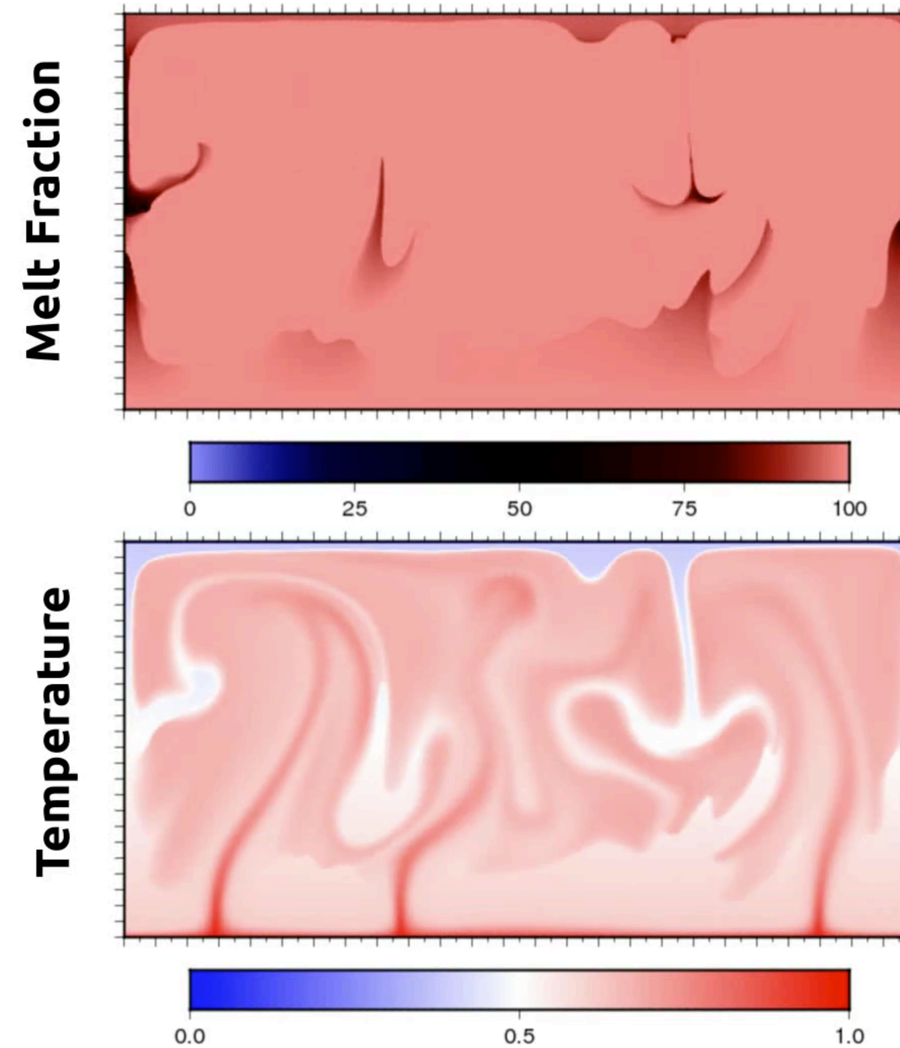
Main governing parameters

Rayleigh number	Buoyancy number	Permeability	Viscosity ratio
$Ra = \frac{\rho g\alpha\Delta T L^3}{\eta_s\kappa}$	$B = \frac{\rho_s - \rho_l}{\rho_0\alpha\Delta T}$	$\epsilon = k_0/L^2$	$\xi = \eta_s/\eta_l$
Convective vigour	*Compositional/phase vs. thermal density contrasts*	*Pore dimension*	

Modelling approach for magma ocean crystallisation & convection

Modelling tool: *Boukaré & Ricard [2017]* finite difference code to solve the two-phase flow averaged equations (conservation of mass, momentum, energy, phase separation, and phase transport)





Advantages

✔ Can model the solidification of a convecting two-phase mixture for all crystal fractions

✔Accounts for melt fusion and crystallisation including latent heat/cooling effects

Current limitations

✔ Cannot handle realistic (large) solid-melt viscosity contrasts or (P,T) variations

✔Advective transport prone to significant amounts of numerical diffusion

✔Sequential and direct matrix inversion scheme computationally prohibitive

➪ limited to coarse grid resolution and unrealistically small Rayleigh number

The Core Proposal

- Can heterogeneities be produced and preserved in the molten mantle, prior to solidification, either through accretionary heterogeneities or core-mantle interaction during core formation?
  - Need to carry out fluid dynamics experiments to investigate the mixing dynamics of such heterogeneities, and whether they can be preserved in the magma oceam regime

- How do molten silicates crystallise to form solids in the mantle?
  - Need to carry out high-P and high-T experiments at all mantle conditions (use LHDAC) to obtain melting relations and phase diagrams of a crystallising silicate melt.

- Accretionary dynamics and primordial differentiation
- Phase equilibria and melting relations in the deep mantle
- Magma ocean – solid mantle dynamical evolution