# 2022 Ada Lovelace Workshop on Numerical Modelling of Mantle and Lithosphere Dynamics

Héviz, Hungary **Workshop booklet** 



28 August - 2 September 2022



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## Foreword and Acknowledgements

Welcome to the 2022 Ada Lovelace Workshop on Numerical Modelling of Mantle and Lithosphere Dynamics! The workshop series was initiated in 1987 in Neustadt an der Weinstrasse, Germany, and workshops usually take place every two years, with the current 3-year interval due to the COVID-19 pandemic. The last workshops were held in Sienna, Italy (2019), Putten, the Netherlands (2017), Oleron, France (2015), Hønefoss, Norway (2013).

The workshops, previously known as International Workshops on Mantle and Lithosphere Dynamics, were renamed in 2018 by the EGU Topical Events Committee in honour of the 19th century English mathematician Ada Lovelace.

The 2022 workshop is co-organised by ETH Zürich and Eötvös Loránd University, Hungary, and takes place at the Ensana Thermal Hévíz Health Spa Hotel in Hévíz, Hungary, about 200 km from Budapest. The meeting is co-sponsored by the European Geosciences Union (EGU), the International Lithosphere Program (ILP) and the ETH Zürich.

## ALW22 Organising Committee:

- Paul Tackley (ETH Zürich, Switzerland)
- Attila Balázs (ETH Zürich, Switzerland)
- Anna Gülcher (ETH Zürich, Switzerland)
- Lászlo Fodor (Eötvös Loránd University, Hungary)
- Lászlo Lenkey (Eötvös Loránd University, Hungary)
- Jeroen van Hunen (Durham University, UK)

The organisers can be contacted at: ada.lovelace.workshop@gmail.com.

In addition to this organisation committee, all members of the Geophysical Fluid Dynamics research group (ETH Zürich) have been helping out with preparation of the workshop, and will take on various organisational tasks during the workshop week.

## ALW22 Scientific Committee:

- Paul Tackley (ETH Zürich, Switzerland)
- Attila Balázs (ETH Zürich, Switzerland)
- Juliane Dannberg (University of Florida, USA)
- Alex Webb (University of Hong Kong, Hong Kong (SAR))
- Ylona van Dinther (Utrecht University, Netherlands)
- Craig O'Neill (Macquirie University, Australia)
- Stephanie Werner (University of Oslo, Norway)
- Shun-ichiro Karato (Yale University, USA)

## Workshop Booklet Editors:

- Timothy Gray (ETH Zürich, Switzerland)
- Kar Wai Cheng (ETH Zürich, Switzerland)
- Anna Gülcher (ETH Zürich, Switzerland)



# **Practical Information**

## **Hotel service**

The hotel helpdesk is open 24 hours a day. Any questions related to your room, your payment, food (dietary wishes), and/or wellness booking should be directed towards the hotel staff. Workshop participants have unlimited use of the hotel's facilities (swimming pool, whirlpool, jin-jang bath, adventure pool, sauna, fitness club). Moreover, the hotel offers workshop participants many wellness treatments with a 20% discount (please schedule outside of workshop programme).

## Breakfast and dinner

Dinner and breakfast are held in the hotel's Tavirozsa restaurant, and both are self-service. Breakfast is open between 07.00-10.00 (note, however, that our programme **starts at 08:30 sharp**), and dinner will be available every evening between 17.30-21.30 (note: our daily schedule runs until 18:30). There will be vegan, vegetarian, and other special options (i.e., gluten, lactose, etc.), which are indicated. For non-standard dietary requirements, please contact the hotel.

## Lunch

Lunch is held from 12:30-14:00 (on Wednesday, from 12:00) near the conference room.

## **Coffee breaks**

We will have a break each morning and afternoon session with beverages and snacks available for all participants. The afternoon break is followed by the student-meet-speakers session.

## Student-meet-speakers

The 30-minute student-meet-speakers sessions are held in the Shakespeare conference room. These sessions are for discussions with and questions to the keynote speakers in an informal setting. Only (graduate / PhD) students and the keynote speakers of that day are present.

## Oral sessions and plenary discussions

Oral presentations will be held in the Shakespeare conference room. The sessions will be in hybrid form with online speakers/participants attending via zoom.

## Poster summary presentations (hybrid)

The poster sessions start off with short presentations aimed to to advertise your poster so that people will want to view it in more detail. These presentations will be held in the Shakespeare conference room (and on zoom), followed by a physical poster session (see below). The length of each promotion presentation should be **30 sec to (max!!) 2 minutes**. You can find the Poster Session Schedule in this booklet. Make sure to have send your presentation PDF or video (optional for online participants) to the organisers well in advance.

## Poster sessions (on-site)

After the summary talks, the physical poster sessions are held in the Haranghy room. You can find the Poster Session Schedule in this booklet. Please hang up your poster either the evening before or in the morning of your assigned poster session day, and please remove your poster again by the end of the day.

## **Online materials**

For online materials and discussions throughout the workshop, we use our own workshop discord server on which each presenter has their own dedicated channel (link provided in e-mail to all participants). In-person presenters should upload a PDF of their poster to their channel on the Discord server. Uploading supporting materials (e.g. slides, a preprint or published paper, a video) is possible. Online presenters may upload any or all of these things (poster, slides, paper, video). The total size will be limited to 100 MB.

## Icebreaker

On Sunday evening, from 21:00-24:00, there will be the Icebreaker reception in the Ciklamen bar.

### Karaoke

The Tuesday evening karaoke event is held in the Brasserie of the hotel from 21:00 until midnight.

#### Wednesday excursion: Geological excursion and wine tasting (12:30-19:00)

The main panoramic highlight of the excursion will be the spectacular view on the perfectly shaped volcanos of the Balaton Highland and Lake Balaton. We will visit Balatongyorok and discuss the evolution of this Miocene-Pliocene monogenetic volcanic field. We will stop at Szigliget and have a look of the castle from the 13th century. We have a look of the geological features of wind erosion at Salfold and finally stop at the winery of Badacsonytomaj and after the wine tasting travel back to Hévíz. **Departure is at 12:30 sharp** (note: only a very quick lunch is possible!). This excursion will be mostly outdoors. Bring **comfortable clothing for active walking** and **protection against the sun/heat** (**cap, sunglasses, sunscreen, etc.**), and a **water bottle**. The winery is inside so a warmer clothing piece may also be handy. Don't forget to bring your camera, too!

### Wednesday excursion: Visit to thermal lake Hévíz (14:45-18:00)

The thermal lake spa of Hévíz is a ~15 minutes walk from the hotel. You may choose your own schedule for this but we will provide a brief talk on the geological aspects shortly after 15:00. The world has innumerable hot water springs and Hungary is one of the countries with the largest thermal water reserves, but none compare to Lake Hévíz at the western tip of Lake Balaton. Covered in waterlilies, the 4.4-ha (11-acre) lake is welcoming all year round: the water temperature does not drop below 24 °C even in winter. The mineral-rich thermal waters, and the traditional treatments using the medicinal mud that covers the lakebed several metres thick, are primarily suited to treating musculoskeletal and rheumatic problems, but the mud's beautifying effects are not to be dismissed either: just one mudpack and your skin will be rejuvenated. Note that the entrance fee is ca. 10 EUR (see online prices).

### Gala dinner and farewell party

On Thursday evening, there will be a special dinner and party for all workshop participants!

### Hungary currency and payments

You'll often find that Budapest is a bargain compared to other European cities because although Hungary is part of the European Union, it does not use the Euro as its currency. The Hungarian currency is the Forint (Ft, HUF), of which there are about 400 to the Euro. Prices, such as hotel rates, sightseeing tours, etc. are often quoted in Euros. Many businesses, even including some select supermarkets accept Euros. Don't forget to check their exchange rates, as you might be better off exchanging your currency first and paying in Forints!

**ATMs** are easy to find in Hungary, and there are many options for exchanging cash. Most often, currency exchange kiosks located in tourist areas or shopping malls offer the best exchange rates. Currency exchange is also available at banks at a surcharge. ATMs dispense Hungarian currency at your bank's daily exchange rate; however, you may be charged a foreign fee on top of the service fees.

**Credit Cards**, such as Visa, Master Card and American Express, are widely accepted. Taxi drivers and public transportation ticket machines in Budapest accept credit cards. Taxi drivers in smaller towns, e.g. in Keszthely or Hévíz probably only accept HUF.

**Tipping** is very much part of the culture in Hungary, and most people will routinely tip. Many restaurants and cafés in Budapest add a 10% service fee, which is usually stated on the bill. If you are unsure, ask your waiter whether or not service was included. If the service fee is not included, unless you were completely unhappy with your service, it is customary to tip 10%-15% of the total bill.

### Departure

On Friday morning, two conference busses will departure from the hotel. The early bus leaves at 08:00 AM, the later bus at 10:00 AM, and both go to the airport. If you have your flight between approximately 12:30-14:30, taking the earlier bus would be a good choice.

**Earlier departure**. We will organise sign-up sheets for these two conference busses. If your flight leaver even earlier (between approximately 11:00 and 12:30), please get in touch with Jeroen van

Hunen, who is organising an even earlier shuttle to the airport.

**Public bus**. If you are not at all in a rush and want to go to Budapest city, we advice to take one of the direct public bus connections instead.

# Workshop Overview

	<b>Sunday</b> Aug 28	<b>Monday</b> Aug 29	<b>Tuesday</b> Aug 30	Wednesday Aug 31	Thursday Sep 1	Friday Sep 2
						Breakfast
		Session 1 Early Earth	Session 2 Crust & lithosphere	Session 5 Subduction & spreading	Session 6 Rheology	& Deparure
08:30		3 keynote talks	3 keynote talks	3 keynote talks	3 keynote talks	
12:30		Coffee break	Coffee break	Coffee break	Coffee break	
		PICO & posters	PICO & posters	Plenary discussion theme 5	PICO & posters	
12:30 14:00		Lunch	Lunch	Geological and scenic excursion	Lunch	
		Session 2 Global Dynamics and Evolution	Session 4 Planets & exoplanets	+ wine tasing	Session 7 Numerical advances	
14:00 - 17:30		2 keynote talks Coffee break	2 keynote talks Coffee break		2 keynote talks Coffee break	
		Students-speakers meeting 1+2	Students-speakers meeting 3+4	Hévíz visit	Students-speakers meeting (5+)6+7	
	Arrival	PICO & posters	PICO & posters		PICO & posters	
17:30 	& check-in	Plenary discussion themes 1+2	Plenary discussion themes 3+4		Plenary discussion themes 6+7	
	Dinner	Dinner	Dinner	Dinner		
21:00 24:00	Icebreaker		Karaoke night		Gala dinner & Farewell party	

# **Daily Programme**

Sunday Aug 28		
all day	Arrival and check-in	
18:00-21:00	Dinner	
21:00-24:00	Ice-breaker reception	

	Monday Aug 29				
Theme 1	Theme 1: Early Earth				
08:30-09:15	Stephen Mojzsis - Observational constraints on early Earth dynamics				
09:15-10:00	Fabio Capitanio - Reconciling craton formation with convective regimes of the early Earth				
10:00-10:45	Stephan Sobolev - Earth's evolution from the Hadean to the present: numerical models versus observations				
10:45-11:15	Coffee break				
11:15-12:30	PICO promotion talks & posters				
12:30-14:00	Lunch				
Theme 2	: Global Dynamics and Evolution				
14:00-14:45	Maxim Ballmer - Long-term thermo-chemical evolution of Earth's mantle				
14:45-15:30	Maëlis Arnould - Some rheological controls on the generation of plate tectonics from mantle convection				
15:30-15:45	Coffee break				
15:45-16:15	Students-speakers meeting				
16:15-17:30	PICO promotion talks & posters				
17:30-18:30	Plenary discussion themes 1+2				
18:30-21:00	Dinner				

	<b>Tuesday</b> Aug 30		
Theme 3: Crust and Lithosphere			
08:30-09:15	Laetitia Le Pourhiet - Long term tectonic modelling: specifities, issues and open questions		
09:15-10:00	Jean-Arthur Olive - Constitutive laws for the brittle lithosphere: Insights from structural geology and experimental rock mechanics		
10:00-10:45	Laurent Husson - Geophysical Biogeography (remotely)		
10:45-11:15	Coffee break		

11:15-12:30	PICO promotion talks & posters			
12:30-14:00	Lunch			
Theme 4: Planets and Exoplanets				
14:00-14:45	Lena Noack - (Exo)planet interior-atmosphere coupling			
14:45-15:30	Ana Plesa - InSights into the interior of Mars: new discoveries and modelling			
15:30-15:45	Coffee break			
15:45-16:15	Students-speakers meeting			
16:15-17:30	PICO promotion talks & posters			
17:30-18:30	Plenary discussion themes 3+4			
18:30-21:00	Dinner			
21:00-24:00	Karaoke			

Wednesday Aug 31							
Theme 5: Subduction and Spreading							
08:30-09:15	<ul> <li>How does a subduction zone initiate at present-day conditions? New insights</li> <li>from a global compilation of Cenozoic events and from numerical studies of the simple set-up of a transform fault undergoing compression <i>(remotely)</i></li> </ul>						
09:15-10:00	Saskia Goes - Volatile recycling in the	e lesser Antil	les Arc (remotely)				
10:00-10:45	Joyce Sim - A two-phase flow perspective on melt transport beneath mid-oceanic ridges						
10:45-11:15	Coffee break						
11:15-12:00	Plenary discussion theme 5						
12:00-	Lunch						
12:30-19:00	Geological and scenic excursion followed by wine tasting	15:00-18:00	Excursion to the Heviz thermal lake				
19:00-21:00	Dinner						

Thursday Sep1						
Theme 6: Rheology						
08:30-09:15	Elvira Mulyokva	ι-	How Microscopic Crystalline Defects Control the Motion of Tectonic Plates			
09:15-10:00	Whitney Behr	-	Rheology of the subduction channel and shear zones from observations <i>(remotely)</i>			
10:00-10:45	Shun Karato	-	Recent Progress in the Experimental (and Theoretical) Study on Plastic Deformation Under Deep Mantle Conditions <i>(remotely)</i>			

10:45-11:15	Coffee break			
11:15-12:30	PICO summaries & posters			
12:30-14:00	Lunch			
Theme 7: Numerical advances				
14:00-14:45	Daniel Kiss - Coupling thermodynamic and thermomechanical codes in Julia to study magmatic processes			
14:45-15:30	Ludovic Räss / Ivan Utkin - Using graphics cards to solve forward and inverse problems in geodynamics <i>(remotely)</i>			
15:30-15:45	Coffee break			
15:45-16:15	Students-speakers meeting			
16:15-17:30	PICO promotion talks & posters			
17:30-18:30	Plenary discussion theme 6+7			
20:00-?	Conference dinner and farewell party			

Friday Sep 2						
07:00-10:00	Breakfast and departure					

## **Poster Sessions Schedule and Presenters**

For the summary live presentations, make sure to have send your PDF material to the organisers well in advance. For the on-site poster presenters: please hang up your poster either the evening before or in the morning of your assigned poster session day, and please remove your poster again by the end of the day.

## Monday morning (11:15-12:30)

### **Early Earth**

Xavier Borgeat (online) Charitra Jain (1) Jeroen van Hunen

### Subduction and Spreading

Marzieh Baes (online) Attila Balázs Ritabrata Dasgupta (online) Daniel Douglas Jiaqi Fang Menno Fraters Pedro José Gea Jódar Iskander Ibragimov Tiphaine Larvet Zhibin Lei Yida Li Valentina Magni Enrico Marzotto Éva Oravecz

## **Monday afternoon** (16:15-17:30)

## **Global Dynamics and Evolution**

Xijuan Bao (online) Heechen Cho (online) Juliane Dannberg J. Huw Davies Matteo Desiderio Valentina Espinoza Mohamed Ismail (online) Ranpeng Li Kang Wei Lim Martina Monaco Gwynfor Morgan James Panton Abigail Plimmer Poulami Roy Nicolas Récalde Neil M. Ribe Arushi Saxena (online) Bernhard Steinberger Zhirui Ray Wang

## **Tuesday morning** (11:15-12:30)

**Crust and Lithosphere** Luuk van Agtmaal Zoltán Erdős Manuele Faccenda Muriel Gerbault Esther Heckenbach Betti Hegyi Andrew Hollyday Elodie Kendall Isabel Kremin Ajay Kumar (online) Kai Li Ziqi Ma (online) Derek Neuharth Sepideh Pajang Alberto Pastorutti (online) Voitěch Patočka Lisa Rummel Alexander C. Rutson Christian Schuler

## Tuesday afternoon (16:15-17:30)

## **Crust and Lithosphere**

Arne Spang Stephanie Sparks Leevi Tuikka

## **Planets and Exoplanets**

Andrea Adams Irene Bernt Kar Wai Cheng Antonio Manjón-Cabeza Córdoba (online) Aymeric Fleury (1) Aymeric Fleury (2) Gregor Golabek Hugo Remise-Charlot Laurine Rey **Tobias Rolf** Antoine Rozel Julia Schmidt Rob Spaargaren Dave Stegman Paul Tackley Jiacheng Tian Sara Vulpius

## Wednesday: no poster sessions

## Thursday morning (11:15-12:30)

**Global Dynamics and Evolution** 

## Venu Gokul

### Rheology

David Bercovici Antoine Demont Jac van Driel Lukas Fuchs Fanny Garel Anna Gülcher Charitra Jain (2) Ágnes Király Mingqi Liu Peter Mora Jyotirmoy Paul Andréa Tommasi Yijun Wang

## **Crust and Lithosphere** Lars Rüpke

### Subduction and Spreading

Manon Pepin Jakub Pokorny Michael Pons Magdala Tesauro (online)

## Thursday afternoon (16:15-17:30)

#### **Numerical Advances**

Nicolas Berlie Thibault Duretz Rene Gassmöller Timothy Gray Lorraine Hwang Boris Kaus Roman Kulakov Albert de Montserrat Navarro Dominic Stemmler Cedric Thieulot David Whipp

## Subduction and Spreading

Noah Hobbs (online) Hee Choi Valeria Turino Yidan Wang Erik van der Wiel Yuan Xie Duo Zhang

# Reconciling craton formation with convective regimes of the early Earth

#### • Fabio A. Capitanio **\*** School of Earth, Atmosphere and Environment, Monash University Clayton, VIC 3800, Australia fabio.capitanio@monash.edu

The sparse geological record provides little clues on how the early Earth worked, and what is the tectonic environment in which the first cratons formed, what does it tell us about the large-scale mantle convection have remained outstanding questions. We gain understanding using numerical models of mantle convection varying temperatures from present-day to Archaean-inferred values reproducing viable dynamics of convective mantle regimes throughout the Earth history. For mantle temperatures comparable to present day, melting is negligible, and the convective regime depends on the strength of the thermal lithosphere. For mantle potential temperatures higher than present-day, high depletion degree and large volumes of mantle residue are formed at low lithospheric strength and a high surface mobility, whereas these are negligible beneath a poorly mobile lithosphere. As dehydrating lithospheric mantle progressively stiffens, a rigid keel forms to stabilise into a craton, while suppressing mobility. The models support an improved understanding of craton formation in the early Earth and support the discussion of the record of the contradicting active Archaean tectonics. The models allow speculations on how representative craton formation might have been of the planet's dynamics, which is addressed through the thermal and tectonics evolution of our planet, in the path towards plate tectonics.

# **Observational constraints on early Earth dynamics**

## • Stephen J. Mojzsis \*

Research Centre for Astronomy and Earth Science, Budapest, Hungary stephen.mojzsis@csfk.org

Comparative planetary studies, combined with increasingly sophisticated geodynamical models linked to geochemical tracers, have done much to inform us about Earth processes before the Hadean-Eoarchean transition around 4 billion years ago. Yet, actual physical chemical evidence for the origin of the oceans and the partition of Earth's crust into discrete continental and oceanic domains comes only from a small inventory of the oldest terrestrial minerals and rocks (dated ca. 4.4 to 3.7 billion years old). The nature of this early record is fickle. Crustal re-working and recycling, whether by (plate?) tectonics, intrinsic (within-crust) or extrinsic (bombardment) melting, along with weathering, denudation and erosion, has effaced it so that there is little concrete to show for the first 150 Myr. Even though tangible lines of evidence serve as critical benchmarks against which numerical models are tested, we seem to have run out of "the oldest rocks" and must extend our reach to exogeology in order to learn more.

There is little doubt that rocky planets form hot. A consequence of post-primary accretion cooling of a silicate planet ought to be the formation of a primary (ultra)magnesian crust such as in the komatiite-basaltic komatiite-basalt series. Once a solid crust formed, mantle convection slowed and water could condense on the surface. Yet when did the surface become cool enough to solidify rock? Did late accretion periodically re-melt the crust?

Indirect evidence from Sm-Nd, Lu-Hf and U-Pb studies shows that substantial silicate differentiation occurred by 4.48 Ga (after the Moon-forming event and postulated Late Veneer), that it has not happened since that time, and the last vestiges of this primary crust appears to have been destroyed by about 3.3 Ga [1-3]. Age, trace element, inclusion mineralogy and isotopic geochemistry of detrital Hadean zircon grains point to continental crust and oceans by ca. 4.38 Ga [4]. I will provide an update on what we know of this time and how the geology of Hadean micro-rocks («1mm in diameter) was just expanded with the discovery of a new zircon locality in the Barberton Greenstone Belt of South Africa [5]. In this context, I will also elaborate on the interval between Moon formation/Late Veneer and the first crust, as well as briefly touch on the source and antiquity of Earth's oceans.

Direct evidence that the continental-oceanic dichotomy of the secondary crust was established by 4 billion years ago comes from studies of quartz-dioritic to tonalitic gneisses, and schists of likely marine sedimentary protolith, preserved in the most ancient gneissic complexes. Calc-alkaline igneous suites like tonalite normally indicate partial melts of hydrated basaltic crust ( $\pm$  garnet), but whether or not their mere presence proves convergent plate tectonics or result from intra-crustal melting and reverse diapirism, continues to be an active topic of debate.

I will conclude with an overview of the earliest record and how this has re-written our view of the Hadean-Eoarchean transition on Earth at about 4 billion years ago from being a hot, dry surface predominantly shaped by impacts, to one defined by relatively benign conditions with liquid water under a dense atmosphere [6].

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# Earth's evolution from the Hadean to the present: numerical models versus observations

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- Charitra Jain GFZ German Research Centre for Geosciences, Potsdam
- Elodie Kendall GFZ German Research Centre for Geosciences, Potsdam

In this study, we address the following three questions with numerical models and compare the results with observations: Was there extensive subduction in the Hadean? When and why did plate tectonics start on Earth? Does coupling of deep and surface processes affect plate tectonics? In particular, we test the hypothesis of Sobolev and Brown (2019 Nature) that major surface erosion events controlled the emergence and evolution of plate tectonics by providing sediments that lubricated subduction interfaces and thus decreased the effective frictional strength of the oceanic lithosphere. We carry out thermo-mechanical numerical modeling using two advanced numerical codes StagYY (Tackley, 2008 PEPI) and ASPECT (Heister et al., 2017 GJI).

For modelling Earth's evolution spanning its entire age, we use StagYY in 2D spherical annulus geometry that generates both basaltic and felsic melts (Jain et al., 2019 Gond.Res.). These compressible models are initialized with mantle potential temperatures ranging between 1750K – 1900K, and employ both diffusion and dislocation creep rheology, as well as a Drucker-Prager friction plasticity. In contrast to the similar previous models (Lourenco et al., 2020 G-cubed), all our models predict intermittent episodes of long-lasting mobile-lid regime and short-lived plutonic-squishy-lid regime in the Hadean and the early Archean (Figure 1), which exhibit extensive subduction leading to rapid production and recycling of the continental crust. These results are consistent with the first measurements of the Rb-Sr isotopes in the komatiite melt inclusions that reveal the presence of Sr87 depleted component with Hadean model age (Sobolev et al., Goldshmidt 2022).

We also implement a drop in the effective friction coefficient of the oceanic lithosphere, simulating the effect of the sediment supply after the emergence of continents in the late Archean and after the Neoproterozoic "snowball Earth" glaciations (Figure 1). Remarkably, our relatively simple reference model, without adjustment of any additional parameters predicts a transition to continuous plate tectonics in the late Archean and reproduces major features of supercontinental cycles inferred from geological observations (Figure 1). These dynamics results from an interplay between secular cooling of the Earth, variable activity of mantle plumes, formation of continents and the lubrication effect of continental sediments. Moreover, the reference model appears to be consistent with the cooling history of the Earth inferred from the petrological observations.

The 2D ASPECT models simulate evolution of global compressible mantle convection and plate tectonics during the last 1 to 2 Gyr of Earth's evolution. Our initial models demonstrate the dependency of the number of subduction zones and plate velocities on changing the frictional strength of the lithosphere, which matches observations.



**Figure 1.** Averaged mobility (grey boxes) and plateness (red curve) functions in the reference StagYY model (lower panel) versus T/P classes and probability of occurrence of metamorphic rocks (upper panel), representing periods of main subduction activity (dashed rectangles). Side panels show snapshots of composition fields of the model in the Hadean (right panel) and at the present day (left panel). Colors at side panels denote compositions: darker and lighter green-

undepleted and depleted pyrolite, violet -basalt-eclogite, orange- TTG. Continents are highlighted by white dashed lines. Letter B with red circle denotes continental break-up point.

# Hadean/Eoarchean tectonics and mantle mixing induced by impacts: a three-dimensional study

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The timing of the onset of plate tectonics on Earth remains a topic of strong debate, as does the tectonic mode that preceded modern plate tectonics. Understanding possible tectonic modes and transitions between them is also important for other terrestrial planets such as Venus and rocky exoplanets. Recent two-dimensional modelling studies have demonstrated that impacts can initiate subduction during the early stages of terrestrial planet evolution-the Hadean and Eoarchean in Earth's case. Here, we perform three-dimensional simulations of the influence of ongoing multiple impacts on early Earth tectonics and its effect on the distribution of compositional heterogeneity in the mantle, including the distribution of impactor material (both silicate and metallic). We compare two-dimensional and three-dimensional simulations to determine when geometry is important. Results show that impacts can induce subduction in both 2-D and 3-D and thus have a great influence on the global tectonic regime. The effect is particularly strong in cases that otherwise display stagnant-lid tectonics: impacts can shift them to having a plate-like regime. In such cases, however, plate-like behaviour is temporary: as the impactor flux decreases the system returns to what it was without impacts. Impacts result in both greater production of oceanic crust and greater recycling of it, increasing the build-up of subducted crust above the core-mantle boundary and in the transition zone. Impactor material is mainly located in the upper mantle, at least at the end of the modelled 500-million-year period. In 2-D simulations, in contrast to 3-D simulations, impacts are less frequent but each has a larger effect on surface mobility, making the simulations more stochastic. These stronger 2-D subduction events can mix both recycled basalt and impactor material into the lower mantle. These results thus demonstrate that impacts can make a first-order difference to the early tectonics and mantle mixing of Earth and other large terrestrial planets, and that three-dimensional simulations are important to obtain less stochastic results, and also to not over- or under-predict the amount of impactor material mixed into the mantle and the time during which a specific tectonic regime acts.



Temperature field of a 2-dimensional simulation due to an impact. On the right panel, we can see cold material being subducted into the mantle caused by the impact

## **Building Archean cratonic roots**

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Geophysical, geochemical, and geological investigations have attributed the stable behaviour of Earth's continents to the presence of their Archean cratonic roots. These roots are likely composed of melt-depleted, low density residual peridotite with high magnesium number, while devolatilisation from the upper mantle during magnatic events might have made these roots more viscous and intrinsically stronger than the convecting mantle.

Several conceptual dynamic and petrological models of craton formation have been proposed. Dynamic models invoke far-field shortening or mantle melting events, e.g., by mantle plumes, to create melt-depleted and thick cratons.Compositional buoyancy and rheological modifications have also been invoked to create long-lived stable cratonic lithosphere. However, these conceptual models have not been tested in a dynamically self-consistent model. In this study, we present global thermochemical models of craton formation with coupled core-mantle-crust evolution driven entirely bygravitational forces.

Our results with melting and crustal production (both oceanic and continental) show that formation of cratonic roots can occur through naturally occurring lateral compression and thickening of the lithosphere in a self-consistent manner, without the need to invoke far-field tectonic forces. Plume impingements, and gravitational sliding creates thrusting of lithosphere to form thick, stable, and strong lithosphere that has a strong resemblance to the Archean cratons that we can still observe today at the Earth's surface. These models also suggest the recycling of denser eclogitic crust by delamination and dripping processes.

Within our computed parameter space, a variety of tectonic regimes are observed which also transition with time. Based on these results, we propose that a ridge-only regime or a sluggish-stagnantlid regime might have been active on Earth during the Archean Eon as they offer favourable dynamics and conditions for craton formation.

# Influence of tectonics on climate, with application to the Marinoan Snowball Earth event

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Tectonic processes such as subduction and seafloor spreading may have a considerable effect on the climate, and the influence of tectonics on extreme climatic events such as the Neoproterozoic Sturtian and Marinoan Snowball Earth periods (with onset times around 726 and 635 Ma, respectively) has been suggested. In particular, the positioning of continents has been proposed to affect climate through variation in albedo effects and latitude of degassing of CO2 and aerosols (Lewis et al., 2003).

Here we present results on the influence of continental latitude on the possible onset of the Marinoan Snowball Earth event. Using the 1-Gyr long paleogeographic reconstruction by Merdith et al. (2021), we examine the correlation between latitude of continents (or more specifically the associated subduction zones) and snowball Earth proxies such as glacial deposits. Using the CLIMBER-3 $\alpha$  modelling tool, we investigate the CO2 threshold needed to trigger a Snowball Earth event, using the most likely plate reconstruction for the Marinoan. Results are compared to more idealised hypothetical plate reconstructions with continents closer to the equator or the pole.

Results show that the latitudinal distribution of subduction zones correlates with some major climate events, including the Snowball Earth events in the Neoproterozoic, suggesting a tectonic influence on these major past climate events. Modelling results (Figure 1) shows that a globally even distribution of continental mass enhances mid-latitude sea ice expansion and increased planetary albedo, thereby increasing the likelihood of a global glaciation. A supercontinent configuration clustered near the south pole is more resistant to a Snowball Earth event. Finally, the Merdith et al. (2021) paleogeographic reconstruction supports the onset of the Marinoan Snowball event but showed greater resistance to equatorial glaciation than the dispersed configuration due to the redirection of tropical ocean gyres and thermal energy to the sea ice front.



Figure: Model results using the Merdith (2021) configuration for the Marinoan period showing a) the land and sea ice fraction at 160 ppm; b) surface heat fluctuations during the 160 ppm SH summer along with the surface wind stress field.

# Some rheological controls on the generation of plate tectonics from mantle convection

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Mantle and lithospheric dynamics of terrestrial planets are intimately related processes. However, despite the large number of numerical models and laboratory experiments on this topic, what finely controls the fact that a planet is in stagnant-lid or in mobile-lid is still unclear. This uncertainty notably arises from the fact that multiple factors, such as lithospheric rheology, and/or compositional heterogeneities, and/or mantle properties, likely play an important role in the generation of plate tectonics.

Global-scale models of mantle convection that self-consistently give rise to plate tectonics most often make use of empirical (such as pseudoplasticity in the lithosphere, also called yield-stress law) and simplified mantle rheological laws (diffusion creep only) [1]. Despite these simplifications, they have demonstrated their ability to statistically reproduce several characteristics of Earth's surface and mantle behavior, such as supercontinent cycles [2], plate-size distribution [3], seafloor age-area distribution [4], surface velocities, heat flow and velocities [5]. However, surface observations of rock deformation at various scales [6], rock-deformation laboratory experiments [7] and regional numerical studies [8] evidence the existence of more complex rheologies and their potential controls on both mantle and surface dynamics.

In this presentation, we will first give an overview of the potential rheological parameters controlling the development of a plate-like behavior in numerical models of mantle convection. Then, we will explore the role of mantle and lithosphere rheology on surface tectonics in numerical models of whole-mantle convection self-generating plate-like behavior. We will focus on the role of strain-weakening and of composite rheology with constant or evolving grainsize, and study how these non-linear effects possibly affect the generation of a plate-like behavior.

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## Long-term thermo-chemical evolution of Earth's mantle

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- Matteo Desiderio and Mohamed Ismail University College London
- Lauren Waszek James-Cook University
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The study of mantle heterogeneity can inform about the evolution and dynamics of terrestrial planets. Heterogeneity is formed by fractionation during melting and crystallization, mainly because the melting temperatures of mantle minerals depend on their composition. Already in their earliest stage, terrestrial planets are thought to evolve through an episode of large-scale melting and fractionation. On Earth, a deep magma ocean has been formed due to the massive energy release during planetary accretion and differentiation. During crystallization of the deep magma ocean at high pressures, bridgmanite is the relevant liquidus phase over a wide range of conditions and may hence be fractionated to form the most ancient heterogeneity in the mantle. Cumulates fractionated in the magma ocean may cover a range of compositions depending on the style of crystallization.

Subsequently, i.e. from the final stages of the shallow magma ocean to the present-day, partial melting in the upper-mantle creates heterogeneity between basaltic (magma) and harzburgitic (residue) end-members. These lithologies are formed near the surface and mixed through the mantle over billions of years. Here, using geodynamic modeling, we show that the distribution of rock heterogeneity in the present-day Earth's mantle strongly depends on their physical properties. For example, while basaltic and harzburgitic materials are stirred by mantle convection, they segregate from each other due to their different densities, particularly in regions of relatively low mantle viscosity. This leads to an enrichment of basalt near the core-mantle boundary, as well as just above the ringwoodite-to-bridgmanite phase transition at 660 km depth. In turn, ancient heterogeneity enhanced in bridgmanite can avoid complete mixing due to its high viscosity. Intrinsically strong material may survive as blobs for large time-scales, as viscous flow is guided around them. The preservation of bridgmanite itself, but also on the density of basaltic materials. For high basalt densities, large thermochemical piles tend to form, which delay mixing of mantle heterogeneity as well as planetary cooling.

The uneven distribution of basaltic material, as well as the survival of ancient materials in the lower mantle, has implications for our interpretation of geochemical and geophysical observations. For example, the materials sampled by mid-ocean ridge or hotspot melting may not be representative of that of the average mantle (i.e., bulk silicate Earth). Seismic data related to acoustic-wave reflections from phase transitions and sharp compositional contrasts provide additional constraints on the distribution of mantle heterogeneity.

## The plume zoo of thermal LLSVPs

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Mantle plumes have been suggested to originate or have a relationship with the Large Low Shear Velocity Provinces (LLSVPs) in the deep mantle. However, the nature of the LLSVPs and the nature of their relationship to plume formation remains under debate. At least two end-members of LLSVPs exist: purely thermal plume clusters and fixed, rigid, thermal chemical piles. While it is challenging to faithfully resolve the multi-scale dynamics of large-scale convection and small-scale plumes simultaneously numerically, laboratory analogs using very viscous fluids and 3-D optical visualization allow us to tackle this question using real-word physics and infinite resolution. We perform a series of experiments in a 40cm x 40 cm x 30 cm plexiglass tank, heated from below. We use scanning Stereoscopic Particle Image Velocity (SPIV) to image the fluid and reconstruct the 3-D velocity field. We start with the purely thermal end-member experiments. We use Lagrangian analysis (FTLE) and cluster analysis (DBSCAN) to track individual plumes and analyze their morphology.

We find that for thermal plume clusters, plume source the bottom thermal boundary layer and show no site preference over time, while plume activity is highly episodic, as plumes depleted the boundary layer. With just temperature-dependent viscosity, plume morphology and behavior are already very rich, including shifting, merging/splitting, branching, deflection, and dying plumes. This rich behavior is in agreement with recent imaging and analysis that prefers plume clusters instead of piles in both global (Davaille and Romanowicz, 2020) and regional (Suzuki et al. 2020) seismic tomography models of the African and Pacific LLSVPs.



Backward Finite-Time Lyapunov Exponent (FTLE) field shown by two contours, the red shows the core of the plumes, and the blue shows the plume boundary.

# Shear Localization in the Lower Mantle: Self-Consistent Solution of Diffusion Creep of Bridgmanite-Ferropericlase Mixture

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Localized deformation is a possible mechanism that may explain the preservation of geochemical heterogeneity in the lower mantle. Experimental studies on diffusional [1] and plastic deformation [2] of the lower mantle minerals showed that ferropericlase (Fp) is significantly weaker than bridgmanite (Br). Due to this strength contrast, it is possible that the lower mantle materials may show strain weakening leading to localized deformation. However, the process of strain partitioning in such a mixture is not well understood. In most previous studies, deformation was assumed to be by dislocation creep (sometimes implicitly). However, there is some hint that deformation in the lower mantle may occur by diffusion creep [3]. One unique aspect of diffusion creep is that the strength of a grain depends on the shape of grain, and, hence, the strength of each grain evolves with strain.

In our previous study [4], we investigated finite-strain deformation of Fp (embedded in Br) by diffusion creep where a Fp grain is embedded in Br matrix. We found that a Fp grain is strain weakened due to the diffusion flux caused by the stress concentration. This tendency is stronger for simple shear than for axial loading. Such strain weakening behavior implies strain localization during the diffusion creep of the Br-Fp mixture. Our next step is to extend this previous study to a Br-Fp mixture with large number of grains to better realize strain localization in the lower mantle.

In this presentation, we report a theoretical development for a solution of diffusion creep of the Br-Fp mixture where many grains are aggregated (polycrystalline). Based on the single grain solution from the previous study using the Eshelby's inclusion theory that relates a surrounding matrix to a local grain, we extend it to multiple Fp and Br grains through self-consistent approach [5]. In this approach, the surrounding matrix is assumed to have a homogeneous property that averages out the properties of all Br and Fp grains (so it is called Homogeneous Effective Matrix (HEM)). This approach allows us to explain that the local weakening affects the overall viscosity of the mixture, which provides more realistic solution. Since the grain's diffusion viscosity continuously changes with deformation (due to its shape change), it is crucial to incorporate this variable viscosity into the diffusion creep solution of Br-Fp polycrystalline mixture. With this approach, we plan to explore the shear localization behavior in Br-Fp mixture at the lower mantle-like conditions.



A diagram for the self-consistent method for a polycrystalline mixture. HEM has homogenized (and uniform) stress ( $\tau^H$ ), strain rate ( $\dot{\epsilon}^H$ ), and viscosity ( $\underline{\eta}^H$ ) of all Br and Fp grains. Each grain's properties ( $\underline{\tau}^I, \underline{\dot{\epsilon}}^I, \eta^I$ ) and HEM properties are simultaneously found in an iterative manner.

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# Evolution of thermochemical structures at the core-mantle boundary controlled by post-perovskite viscosity and subduction history

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The chemical and thermal heterogeneity of the lowermost mantle is highlighted in many observations, such as seismic wave speed, plume compositions, or the geoid. While the last decades have brought substantial advances in knowledge in particular about the large low shear velocity provinces below Africa and the Pacific, there are still numerous open questions about their origin, development and stability. In particular, it remains unclear what material they are made of (predominantly primordial vs. recycled), and modeling studies come to different conclusions about how easily basaltic crust can segregate from subducted slabs and be incorporated into these reservoirs. Furthermore, there are questions about their longevity: On the one hand, it has been suggested that they have remained in their present location for hundreds of millions of years, on the other hand their location has been suggested to change in response to where subduction occurs.

We address these questions using 2D and 3D numerical modeling of the interaction between subducted slabs, the core-mantle boundary, and rising mantle plumes. Specifically, we take into account the influence of the viscosity reduction induced by the presence of postperovskite on the segregation of oceanic crust from subducted slabs, and we model the interaction of subducted slabs with thermochemical piles at the core-mantle boundary throughout the past billion years of Earth's history.

Our models show that the rate at which basaltic crust can accumulate in chemical structures at the core-mantle boundary is controlled by a complex interplay of the post-perovskite viscosity and the crustal thickness. If lower mantle slabs have the same crustal thickness as at the surface, a low post-perovskite viscosity decreases basalt accumulation in piles because recycled crust is carried upwards by plumes more efficiently. The more the crust thickness when crossing from the surface to the more viscous lower mantle, the more low viscosity facilitates pile growth, since the higher influx of dense basaltic material can suppress the rise of plumes. In addition, we show that thermochemical piles change in location, shape and number throughout the supercontinent cycle. At times where subduction location changes frequently, thermochemical piles fork or split up. Conversely, stable subduction zones (such as in the immediate past) lead to large and stable piles. Our results indicate that thermochemical structures at the core-mantle boundary fluctuate more than previously thought and might have looked very differently throughout Earth's history.



Figure 1: Left: 3D global convection model tracking the evolution of thermochemical structures. Right: Models of basalt segregation, with either very low (top) or high (bottom) accumulation of basalt in thermochemical structures.

# Investigating the influence of "660" phase transition on subduction using dynamic extended Boussinesq approximation models

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Whether and how subducting slabs penetrate through the upper / lower mantle boundary is incompletely understood. This will have a big bearing on Earth's thermal and chemical evolution. For example early work showed that if the Clapeyron slope of the ringwoodite to bridgmanite and ferropericlase phase transition, which occurs at around 660 km depth in mean mantle, (so called "660" going forwards) was sufficiently negative, then slabs could be prevented from passing through. Is this the case for dynamic models? Is this the case when the latent heat of the phase transition is also considered? How will the slabs behave as a function of the thermal structure (age) of the subducting and overriding plates?

To investigate these questions we have undertaken 2D Cartesian models of subduction with a similar geometry to Garel et al., (2014). These simulations were undertaken using the adaptive code Fluidity (Davies et al., 2011), using an unstructured grid. While the Garel et al. (2014) models used the Boussinesq approximation (BA), the models here are using the extended Boussinesq approximation (EBA). This means that the latent heat effect of phase transitions (included using the method of Christensen and Yuen, 1985) can be included self-consistently. We have investigated many models, including models within the BA with Clapyeron slope of 660 varying from 0 to -2 to -4 MPa/K values. We have then undertaken models in the EBA with 660 Clapyeron slopes of 0 and -2 MPa/K. The models are undertaken for a range of initial ages of the subducting and overriding plates at the trench.

In all the models, slabs subducted to the lower mantle. The models with young subducting plate ages frequently subducted vertically and could incur some folding as the slabs penetrated the more viscous lower mantle. While for older subducting plates they can remain bent, and frequently the trench can rollback giving a more inclined orientation to the subducting slabs. The influence of the Claperon slope is modest, and the difference between the BA and equivalent EBA simulations is minor. This work shows that for current best estimates of the 660 Clapeyron slope slabs will penetrate into the lower mantle. The behaviour of the subducting slabs as a function of the thermal structure of the subducting and overriding plate is presented through regime diagrams. A range of morphologies are represented.



Figure Caption – Regime Diagrams as a function of initial plate age at the trench, for subduction models in the Extended Boussinesq Approximation with varying Clapeyron slope for the '660' phase transition. The Clapeyron value is 0 MPa / K on the left hand side, and -2 Mpa / K on the right hand side.

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## The interplay between recycled and primordial heterogeneities: constraints on Earth mantle dynamics via numerical modeling

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A quantitative understanding of Earth's deep compositional structure remains elusive. Geophysical and geochemical observations illuminate heterogeneous features on various scales in the lower mantle: however, the origin and interaction of such heterogeneities are not yet fully explained in the context of global mantle dynamics. Conversely, numerical geodynamic models predict a wide range of viable scenarios of mantle convection and heterogeneity preservation. In the "marble cake" end-member mantle model, slabs of Recycled Oceanic Crust (ROC) are subducted and deformed but never fully homogenized in the convecting mantle. In the "plum pudding" model, MgSiO<sub>3</sub>-rich primordial material may resist convective entrainment due to its intrinsic strength. Only few geodynamic studies have explored the effects of subducted ROC properties on mantle dynamics while also accounting for the influence of primordial heterogeneity. Furthermore, predictions from numerical models need to be tested against geophysical data. However, current imaging techniques poorly resolve the lower mantle and may be unable to distinguish between both end-member models above.

Here, we use the finite-volume code StagYY to model mantle convection in a 2D spherical-annulus geometry. We investigate the style of heterogeneity preservation as a function of two parameters: the intrinsic density and the intrinsic strength (viscosity) of basalt at lower-mantle conditions. Additionally, we employ the thermodynamic code Perple\_X and the spectral-element code AxiSEM to compute, respectively, seismic velocities and synthetic seismograms from the predictions of our models.

We obtain two main regimes of mantle convection: low-density basalt leads to a well-mixed, "marble cake"-like mantle, while dense basalt aids the preservation of primordial blobs at mid-mantle depths as in a "plum pudding". Intrinsically viscous basalt also promotes the preservation of primordial material. These trends are well explained by smaller convective vigour of the mantle as intrinsically dense (and viscous) piles of basalt shield the core. In order to test these model predictions, we convert model temperatures and compositions to thermoelastic properties for two characteristic models of each regime. These are then used to compute synthetic seismic velocity models, through which we simulate wave propagation using AxiSEM. Finally, we discriminate between these two end-members by comparing statistical properties of the corresponding ensembles of synthetic seismograms. Our results highlight how the interaction of mantle materials drives the long-term thermochemical evolution of terrestrial planets. Furthermore, they provide a framework for relating the style of heterogeneity preservation in the Earth's lower mantle with specific features of the seismic waveforms.

## Unravelling the crustal and upper mantle contributions to the Indian Ocean Geoid Low based on constrained potential field modelling

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he Indian Ocean Geoid Low (IOGL) located at the south of India in the Central Indian Ocean is one of the most intriguing geophysical features on Earth. It is characterised by a long wavelength geoid depression of -106 metres centered at 79°E and 5°S. The anomaly reduces by 50% at a radial distance of 2500 km from the centre. There is significant debate about the causative factors contributing to the IOGL as the depth and nature of the sources remain enigmatic. We attempted to understand the contribution of crustal and upper mantle density related to the IOGL using joint analysis of topography, geoid, gravity data along with available seismic tomographic models. Spectral decomposition of the geoid anomalies reveals that only a small fraction (up to 10%) of the IOGL is due to mass anomalies lying within the crust and the upper mantle ( <700km). Crustal and upper mantle density structures were determined using 3-D gravity inversion along with the SL2013sv tomographic model. The geoid response of these density structures up to 700 km are then compared with degree-10 residual geoid anomaly. This comparison suggests the presence of density sources within the sub-lithospheric mantle. Joint gravity-geoid modelling of these low-density anomalies confirms that the total contribution of density structure up to the upper mantle depths (700 km) accounts for only 10% of the IOGL whereas the remaining part is primarily caused by mass anomalies in the lower mantle.

## Inference of Recent APM Changes from the Analyses of RPM Changes

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Since the dawn of the Plate Tectonics theory, important efforts have been put towards reconstructing the past motion of plates. Mapping of the ocean-floor magnetization, for instance, has provided remarkable estimates on the relative spreading between adjacent oceanic plates. Combining these measurements into plate circuits allows one to workout the relative plate motion (RPM) of non-adjacent plate pairs or even plates sharing a convergent/collisional margin. These reconstructions can be then tied to a deep-Earth absolute reference frame by resorting to hotspot tracks left by mantle plumes. Unlike the reconstruction of recent relative motions – who relish today of an unprecedented temporal spacing of 1-2 Myr – the resolution and precision of plumebased absolute plate motions (APM) is often limited by the complex and sparse hotspot tracks found in e.g. slow-spreading regions.

On the other hand, the kinematics of tectonic plates lacked a mechanism to account for the driving and resisting forces that govern such motion. The work of Forsyth and Uyeda [1975] – likely the most influential on this matter – sparked interest on shallow-seated forces, e.g. slab-pull or ridge-push. Additionally, recent numerical simulations have provided a better understanding of the forces acting at the base of the plate [Stotz et al., 2018]. However, computing most of these forces requires knowledge of the plate's motion rate (i.e., APM estimates).

Taking advantage of the tools developed by Iaffaldano et al. [2014], we extract the recurrence with which a change in the plate's relative motion is likely to happen. By combining the likeliness of several neighboring plates, we can assess whether any of them is likely to feature an APM change through geological time. By extracting changes in APM from RPM sequences, we are able to preserve the high resolution of RPMs. This is of key relevance, as changes in plate motions – and the forces acting upon them – can occur within only a few Myr [Iaffaldano and Bunge, 2015] (i.e. shorter intervals than the current resolution that plume-based APM estimates can achieve [Wessel and Kroenke, 2008]). With this approach we are able to provide useful estimates on the Quaternary/Neogene kinematic history of plates, which are essential for future studies on the plate-driving forces behind.

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### Fractional crystallization of the Basal Magma Ocean: The consequences on present-day mantle structure

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Constraining thermal evolution for the deep interior of terrestrial planets is substantial to understanding their evolution as a whole. Thermal evolution is controlled by stages of large-scale melting, or magma oceans -due to the energy released during accretion, differentiation and radioactive decay of heat-producing elements- and crystallization of this melt. Thus, exploring the crystallization sequence of the Basal Magma Ocean (BMO) is vital for understanding the thermal evolution of the planets and their related structures in the lower mantle. Previous work shows that a FeO-enriched molten layer or basal magma ocean (BMO) is stabilized at the core-mantle boundary for a few billion years. The BMO itself is expected to freeze by fractional crystallization (FC) because it cools very slowly, FC always yield a highly iron-enriched BMO and last stage cumulates. Other crystallization mode could be dominated and has not yet been systemically explored.

To explore the fate of the BMO cumulates in the convecting mantle, we explore 2D geodynamic models with a moving-boundary approach. Flow in the mantle is explicitly solved, but the thermal evolution and related crystallization of the BMO are parameterized. The composition of the crystallizing cumulates is self-consistently calculated in the FeO-MgO-SiO<sub>2</sub> ternary system according to Boukaré et al. (2015). In some cases, we also consider the effects of Al2O3 on the cumulate density profile. We then investigate the entrainment and mixing of BMO cumulates by solid-state mantle convection over billions of years as a function of BMO initial composition and volume, BMO crystallization timescales, distribution of internal heat sources, and mantle rheological parameters (Ra# and activation energy). We varied the initial composition of BMO by manipulating the molar fraction of FeO, MgO, and SiO<sub>2</sub> -based on published experiments- to model different BMO-compositions: Pyrolitic composition, After 50% crystallization of Pyrolitic composition Caracas et al. (2019), and Archean Basalt.

For all our model cases, we find that most of the cumulates (first 90% by mass) are efficiently entrained and mixed through the mantle. However, the final 9% of the cumulates are too dense to be entrained (either fully or partially), and rather remain at the base of the mantle as a strongly FeO-enriched solid layer. We highlight that this inevitable outcome of BMO fractional crystallization is inconsistent with the geophysical constraints. Our results suggest that a BMO was either very small initially which is tested in our study and the results are only consistent with the geophysical constraints when BMO volume less than or equal to 100 km, or did not crystallize by FC. An alternative mode of crystallization may be driven by an efficient reaction between a highly-enriched last-stage BMO with the overlying mantle due to chemical disequilibrium.

Phase transitions may have induced plume and slab stagnation in Earth's past: modeling with a new entropy method and viscoplastic rheology

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Mineral phase transitions influence mantle flow through their effect on buoyancy and latent heat. The deflection of the transition depth caused by their Clapeyron slope can contribute either a positive or a negative buoyancy force to mantle flow. The latent heat consumed or released during phase change can lead to abrupt changes in temperature across phase transitions and partially compensates the buoyancy effect. During Earth's secular cooling, different phase transitions might have controlled mantle dynamics, implying a change in convection patterns. Therefore, it is important to incorporate the thermodynamic effects of realistic phase transitions to properly explore their influence on mantle convection throughout Earth's history. Our study applies a new numerical technique, which reformulates the energy conservation equation in terms of specific entropy instead of temperature. This allows us to accurately include the latent heat effect for mantle temperatures away from the average geotherm, and therefore better captures the effects of phase transitions than previous studies.

We set up 2-D models with the geodynamics software ASPECT, using thermodynamic properties computed by HeFESTo, to model global convection with a broad range of core-mantle boundary temperatures and starting mantle adiabats. We have demonstrated the applicability of the new formulation through a series of simplified purely viscous models, which capture the layering of plumes induced by the wadsleyite to garnet + ferropericlase endothermic transition (between 420-600 km depth and over the 2000-2500 K temperature range). Our models show that this phase transition causes a large-scale and long-lasting temperature elevation in the depth range of 500–650 km if the initial adiabat is 1800 K and higher. This result implies that mantle convection may have been partially layered early in Earth's history. Furthermore, we have created models that incorporate a realistic viscosity profile and a visco-plastic rheology to better reproduce selfconsistent plate tectonics and Earth-like subduction morphologies. They show that the phase transformation from ringwoodite to bridgmanite + ferropericlase at 660 km depth, together with a steep increase in viscosity, can partially stagnate a slab between 600-800 km depth, depending on its thickness and rate of slab retreat. These models will serve as a starting point to explore how phase transitions have impacted layering of convection and the Earth's thermal evolution throughout its history.

## Gravitational Collapse of a Metal-Silicate Mushy Layer at the Core-Mantle Boundary

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The core-mantle boundary (CMB) is one of the most stable interfaces inside the Earth owing to the large density and viscosity contrasts. Despite significant differences in chemical and physical properties between the core and mantle, the possible mechanisms in which the core and mantle can interact is becoming an active area of research. Detection of chemical signatures from the CMB can provide an unprecedented glimpse into our planet's deep interior and ancient past as several isotopic and elemental anomalies in ocean island basalts (OIBs) have been proposed as core tracers (e.g.  ${}^{3}\text{He}/{}^{4}\text{He}$ ,  $\mu^{182}$ W, D/H). However, the process(es) by which particular chemical signatures from the core are conveyed into the mantle still remain uncertain. We propose a new hybrid mechanism that results from a collaborative feedback between dynamic topography, porous infiltration of liquid metal into submerged rock, gravitational collapse of a rheo-logically weakened metal-silicate mush, and draw-down of additional rocks from above in the induced small-scale mantle circulation. The grain-scale intrusion of liquid iron into mantle rocks at the CMB will allow chemical exchange to take place within the metal-silicate mush, while viscous compaction of the silicate matrix during gravitational spreading of the mushy mixture will expel liquid metal back into the core. This allows the chemically reacted rock to carry a "taste" of the core into the shallow mantle. Using a mantle convection model coupled to the gravitational spreading of a thin layer at the CMB, we show that the induced mantle circulation due to the gravitational collapse of the layer becomes comparable to buoyancy-driven mantle flow when the viscosity of the mushy layer is reduced to values  $10^5$  times smaller than the overlying mantle. We also derive a scaling law that relates the enhancement of downwellings into the mushy zone with the viscosity contrast and aspect ratio of the mushy layer.

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 (a) Schematic illustration of the hybrid mechanism. h represents the thickness of the mushy layer, which is similar to the amplitude of dynamic topography. Solid black arrows illustrate downwelling mantle flow that induces dynamic topography while dashed arrows illustrate flows due to the gravitational collapse of the metal-silicate mush. (b) Flow chart of the hybrid mechanism explicitly showing the feedback loop.

## Recycled basaltic material in mantle plumes explains the appearance of the X-discontinuity in the upper mantle: 2D geodynamic numerical models

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Mantle plumes have a widely known role in recycling materials from the deep Earth, but the quantities of the latter are not well constrained. Important indications come from seismic discontinuities like the X-discontinuity, which is particularly apparent around 300 km depth beneath the Hawaiian hotspot and is interpreted to be the coesite—stishovite phase transition. Seismological observations argue that, for the X-discontinuity to be observed, 40% or more eclogitic-rich recycled material needs to be present. However, classical geodynamics studies indicate that a mantle plume can only carry up to 15-20% denser recycled material to the surface, in order to maintain the necessary positive buoyancy to rise.

To resolve this controversy, we run two different sets of 2D geodynamics numerical models employing the mantle convection code ASPECT. In our first series, we model the recycled material within the plume conduit in the form of discrete heterogeneities with diameters of 30—40 km, such that they do not mix with the background pyrolite and material segregation is allowed. Depending on the background viscosity, we observe three regimes. For its lowest values, the heterogeneities are too dense to be entrained: basalt segregation is therefore directed downwards and no accumulation is attained. Conversely, at the highest viscosity values, the heterogeneities rise together with the background. For intermediate viscosities, we detect cyclical ponding and material accumulation around and above the 410 km depth global discontinuity, with occasional peaks up to 40-50% recycled material.

To further explore the effect of the entrained basalt on plume dynamics we extend our models, now assuming mixing between the mantle and the recycled materials. We also overcome limitations of our previous study by accounting for the energy balance, allowing the velocity to develop dynamically and the plume to spread laterally.

These regional models feature a background mantle — made up of 82% harzburgite and 18% basalt — and mantle plumes with 1-15% additional basalt. Our preliminary results show that, in the range of plume excess temperatures between 200—300 K, the plume can still rise with up to 30% recycled basaltic material in the whole model, provided that it is hot enough to counterbalance the increased density.

Our models suggest that mantle plumes have the potential to accumulate higher percentages of denser material than previously thought. These results also provide a viable mechanism to explain the regional appearance of additional mantle phase transitions like the X-discontinuity.

### **Constraining Mantle Circulation Models with Seismic Structures**

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The interplay of seismological observations, conceptual models, and numerical modelling has driven much of the progress in our understanding of the deep mantle; most notably in the use of the radial 1D seismic discontinuity structure in early discussions about layered convection, and the conversion of geodynamic model results into seismic velocities that are then filtered and compared to published tomographic models. Comparisons between geodynamic and tomographic models have been particularly popular due to the large amount of data contained in tomographic models and the potential for informative visual comparison.

However, modern seismology produces a wide array of datasets that can be compared against the latest numerical models. These observations include those made using Receiver Functions (e.g. Cottaar and Deuss, 2016) and SdS travel-times (e.g. Shearer and Masters, 1992) to investigate the topographies of transition zone discontinuities, radial 1D velocity structures (e.g Dziewonski and Anderson, 1981) in addition to full tomographic models. In this presentation, we will use some of these datasets to explore current ideas on mantle dynamics.

We post-process temperature, pressure, and composition fields generated from Mantle Circulation Models run in TERRA (Baumgardner, 1983) to produce synthetic seismological datasets. We will present early results considering the topography of mantle transition zone discontinuities. We will compare these modelled outputs to published datasets to discriminate between conceptual models, including the potential role of akimotoite phase transitions during slab entry into the lower mantle (e.g. Cottaar and Deuss, 2016), the significance of an iron-spin transition in the lower mantle, and the plausibility of various rheological profiles.



Figure 1:

Summary figure of questions of interest for programme of research presented; the importance of transition zone phase boundaries, the role of akimotite phase changes in colder parts of the mantle, the importance of the iron spin transition and the asthenosphere.

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### Heat producing elements and mantle heterogeneity in geodynamic models

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The chemical heterogeneity introduced into the mantle by the subduction of oceanic crust may contribute to the formation of the seismically observed large-low velocity provinces (LLVPs). However, heat producing elements (HPEs) concentrated in oceanic crust may limit the longevity of recycled material in the lower mantle. The fingerprint of the introduced heterogeneity is realised in the range of geochemical compositions observed in mantle derived rocks such as mid-ocean ridge basalts (MORBs). Uranium is a HPE of particular interest which, together with Pb, forms a decay system which can be used to trace the average age of mantle heterogeneity. The two elements are fractionated from one another by multiple processes, the sum of which is reflected in the <sup>207</sup>Pb/<sup>204</sup>Pb - <sup>208</sup>Pb/<sup>204</sup>Pb array. We show that a combination of preferential removal of Pb from the subducting slab and recycling of U from the continental crust after the great oxygenation event at 2.4 Ga are required to explain the distribution of Pb isotope ratios measured in oceanic basalts. The additional internal heating provided by recycling U is shown to have little effect on how oceanic crust accumulates at the CMB. However, in simulations with spatially heterogenous internal heating rates driven by the concentration of HPEs, accumulations of recycled oceanic crust are more readily destabilised than simulations with homogeneous heating rates. This highlights the importance of accurately modelling internal heating when investigating the chemical heterogeneity of the mantle.



Visualisations of the bulk composition field for 3 mantle convection simulations with iso-surfaces drawn around C=0.9. In each case parameters and initial conditions are identical except for no U recycling in b) and homogeneous heating rate in c). a) Piles of recycled oceanic crust form but before present day are destabilised and move away from the core-mantle boundary (CMB). b) Uranium is not recycled from the continental reservoir but piles still de-stabilise before present day. c) When the internal heating rate is distributed homogeneously throughout the mantle, piles of recycled oceanic crust persist at the CMB to present day.

# Constraining the relationship between mantle convection and supercontinent cycles

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For decades, researchers have studied supercontinents and their important implications for the evolution of climates and biological systems through geological time (Nance et al. 2014). Despite this, the mechanisms which control the breakup and amalgamation of these supercontinents remain enigmatic.

We consider a mantle convection 'cycle' (figure 1), comprising downwellings, deep mantle structures, upwellings, and the continents. This cycle encompasses the critical features and processes involved in the breakup and assembly of supercontinents. Whilst it is possible to constrain the present-day geometries and localities of mantle features using seismic tomographic models, understanding the mechanisms and mantle dynamics which give rise to them is more complex. We aim to constrain the degree of feedback between the surface and CMB boundary layers by modelling the mutual interaction of their respective instabilities, slabs and plumes.

As such, we present the following research questions:

- On what timescales do LLSVPs respond to subduction and what are the possible implications of this for upwellings?
- How much stress is exerted on a supercontinent by slab pull if the slab (a) stalls at the transition zone, (b) penetrates the upper region of the lower mantle, or (c) penetrates straight through to the CMB?
- What role does mantle inheritance play in the supercontinent cycle? Can each cycle be considered in isolation or are the structures predetermined by previous cycles?
- How has the feedback between the surface and CMB changed since the onset of plate tectonics, specifically through the pre-Wilson Cycle era?

We utilise the 3D mantle convection code, TERRA (Baumgardner 1983), to model the interaction between slabs subducted around the edges of supercontinents and deep mantle structures.

Our initial models will be preconditioned to have thermal and/or chemical anomalies at the CMB to reflect LLSVPs. We'll track and measure the sinking times of slabs with varying physical properties and geometries throughout the mantle. Sinking times will be measured to the top surface of our thermochemical anomalies and to the CMB. Slab buoyancies and sizes, as well as radial viscosity profiles within the mantle are varied to constrain the implications of each parameter. Subsequently, we will track the centre of our thermochemical piles to understand the timescales on which they interact with downwelling slabs and ask, when considered in relation to proposed plume ascent times, whether this cycle can occur within the lifetime of a single supercontinent.



Figure 1: Schematic diagram of the key elements comprising a mantle convection 'cycle' as it refers to supercontinents.

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# Modelling seismic anisotropy of Earth's lower mantle in a 3D plume geodynamic setup

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Seismic anisotropy is an observation that is believed to yield information on the flow pattern in the mantle. There are many studies of anisotropy in the upper mantle; however, the lower mantle is still underexplored, due to problems in seismic imaging and complexities of modelling of flow laws of different minerals. In this study, we investigate the integrated strain on particles moving with the flow in a 3D whole mantle geodynamic plume model using the finite element code ASPECT. Then we use the texture development code D-Rex coupled with ASPECT to model the crystallographic/lattice preferred orientations (CPO/LPO) of Bridgmanite and post-Perovskite separately which are the dominant mineral phases in the lower mantle. We predict the elastic tensors and the maximum and minimum eigenvectors of elastic tensors of each mineral phase. We find that the inside of the plume is more anisotropic than the surrounding. We also see that the anisotropy becomes higher with higher values of integrated finite strain for both of the mineral phases.



Figure 1: (a) Plume upliftment at 25 Ma shown as high temperature anomaly with integrated finite strain as particle property; (b) No CPO outside of the plume; (c) CPO generation and high anisotropy inside the plume

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## **Understanding Noble Gases in the context of Mantle Dynamics**

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Noble gases provide a set of constraints that help us to understand Earth's mantle dynamics and thermal evolution. Amongst these noble gases, helium (He) and argon (Ar) are of particular interest as radiogenic isotopes are produced by the main Heat Producing Elements (HPEs) within the mantle: <sup>235,238</sup>U, <sup>232</sup>Th for <sup>4</sup>He and <sup>40</sup>K for <sup>40</sup>Ar. High He ratios sampled by Oceanic Island Basalts (OIBs) suggest a preserved unprocessed source of primordial 3 He. Current atmospheric Ar concentrations indicate that only half of the radiogenic Ar has been outgassed, based on the initial budget of 40 K. Geochemists initially proposed a layered mantle to explain noble gases data, however seismic tomographic models strongly support whole mantle convection (Albarède & van der Hilst 2002).

Preserving compositional and geochemical heterogeneity within the convecting mantle is imperative to explain both He and Ar observations. However, the melting process that creates the heterogeneity, contributes to heat transfer, and controls outgassing, is crucial but not fully understood and could significantly impact noble gases ratios. The aim of this project is to build a model that is consistent with geophysical and noble gases data. We focus on three major processes that are critical to the noble gases problem; the preservation of geochemical heterogeneity, melting, and outgassing.

We investigate this problem with numerical simulations using the 3D finite-element code, TERRA (Baumgardner 1983), implementing particle tracking for a composition dependent buoyancy and isotopic tracing in a spherical shell (Van Heck et al. 2016). We distinguish two categories of models: mantle convection models (in which both the top and bottom boundary layers are free-slip surfaces) and mantle circulation models, which implement plate motion reconstructions to the surface boundary layer, hence reproducing more Earth-like behaviour.

Initially, we will investigate how melting is driven in TERRA simulations; whether it is predominantly driven by fertile compositions or temperature excesses for each category of model (i.e. convection or circulation). Also, we vary the input of HPEs by implementing various published K/U ratios to investigate the potential impacts on both dynamics and noble gases isotopic ratios. Since outgassing efficiency could also have an impact on atmospheric Ar and keeping primordial He within the mantle, implementing a depth dependent outgassing is also considered. Varying the buoyancy number of subducted oceanic crust allows us to increase residence time within the deep mantle and thus preservation of high He ratios. However, such material would have to have a seismic signature similar to the observations.

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## Scaling of Free Subduction on a Sphere

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Because the earth's tectonic plates are doubly curved shells, their mechanical behavior during subduction can differ significantly from that of flat plates. We use the boundary-element method (BEM) to study free (gravity-driven) subduction in axisymmetric and 3-D geometry, with a focus on determining the dimensionless parameters that control the dynamics. The axisymmetric model envisions a shell with thickness h and viscosity  $\eta_1$  subducting in an isoviscous planet with radius  $R_0$  and viscosity  $\eta_0$ . The angular radius of the trench is  $\theta_t$ . Our implementation of the BEM employs a new point-force Green function that satisfies free-slip boundary conditions everywhere on the surface of a unit sphere. Scaling analysis based on thin-shell theory reveals two key dimensionless parameters. The first is the 'flexural stiffness'  $St = (\eta_1/\eta_0)(h/l_b)^3$ , where  $l_b$  is the 'bending length', or the sum of the slab length and the length of the seaward flexural bulge. St controls whether subduction is rate-limited by the viscosity of the ambient mantle ( $St \gg 1$ ) or by the shell's own viscosity (St  $\ll$  1). The second, the 'sphericity number'  $\Sigma = (l_b/R_0) \cot \theta_t$ , measures the importance of spherical geometry. Its definition implies that small plates have greater sphericity than large ones, and that a hemisphere with  $\theta_t = 90^{\circ}$  ( $\Sigma = 0$ ) subducts like a flat plate, a result that we verify by comparing spherical and Cartesian simulations. We find that sphericity reduces the sinking speed of a subducting slab by up to 35% for small plates such as the Cocos and Philippine Sea plates, and 7% for a large plate like the Pacific plate. However, sphericity increases the hoop stress resultant (the key quantity controlling the growth rate of buckling instabilities) by up to 240% for small plates. Turning to 3-D geometry, we examine the linear stability of shells to longitudinal perturbations corresponding to buckling. The most unstable wavenumber n is a strongly increasing function of the lower mantle/upper mantle viscosity ratio  $\lambda$ , providing a possible explanation for the characteristic 'scallop' wavelength of trench segmentation on earth. We explain the systematics of  $n(\lambda)$  by means of a simple analytical Rayleigh-Taylor instability model.

## Global mantle flow models constrain balance of plate-tectonic forces by matching surface motions

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Mantle convection models based on geophysical constraints have provided us with a basic understanding of the forces driving and resisting plate motions on Earth. However, previous studies have come to different conclusions on the balance of the underlying forces that generate the observed surface deformation. Moreover, existing models use a simplified plate boundary geometry, and the impact of this geometry on global plate motions remains uncertain.

To address this, we develop global instantaneous 3-D mantle convection models and quantify the relative importance of the different components of the mantle–plate system on the surface plate motions. Our models have a heterogeneous density and viscosity distribution inferred from the LLNL-G3D-JPS tomography model and a temperature model that includes well-resolved slabs and lithospheric structure. We prescribe weak plate boundaries based on four different plate boundary configurations, either using dipping shear zones and open plate boundaries, or vertical shear zones and closed plate boundaries. To resolve the strong variations in viscosity, we use adaptive mesh refinement such that the uppermost mantle has a minimum cell size of 15 km.

We find that models with open plate boundaries that are 4 to 5 orders of magnitude weaker than the surrounding lithosphere, and low asthenospheric viscosities between 5e17 Pas and 5e18 Pas achieve the best fit to the observed GPS data both in direction and speed of plate motion. In particular, the best fitting model has open and dipping weak shear zones based on Bird's plate model (Bird, 2003) only in the oceans (at subduction zones and mid-oceanic ridges), while deformation is more distributed within continents. This result suggests that plate boundaries are not uniformly weak everywhere and are better described by using stronger plate boundaries within the continents compared to the oceans. Our best-fit model has a directional correlation of 95% and a global point-wise residual of 2.5 cm/year with respect to the GPS velocities. Models without asthenospheric and lower mantle heterogeneities retain on average 25% and 50% of the plate speeds, respectively, emphasizing the importance of slab pull in the uppermost mantle as a driving force.

Our models advance our understanding of the balance and physical mechanisms of plate driving forces and show the importance of plate boundary geometry for the direction and speed of plate motions. In addition, they can serve as a starting point to improve the predictions of the current generation of global plate models.



Figure 1: The effective viscosity field for our reference model showing the equatorial plane and the plate boundaries in red. NA: North American plate, MAR: Mid-Atlantic Ridge.

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### The cause of the deepest geoid low on Earth

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While the geoid is often displayed with respect to the "reference ellipsoid", with its deepest low south of India, it is geodynamically more appropriately displayed with respect to the hydrostatic equilibrium ellipsoid, in which case the deepest low is beneath West Antarctica. In a similar region, there is also a residual topography high. This region is characterized by thin lithosphere, and a mantle plume has been suggested beneath. Hence upper mantle viscosity could be regionally reduced, allowing for faster rebound than elsewhere upon melting of the West Antarctic Ice Sheet (WAIS) which is one of the tipping elements of the global climate system. To study the possible causes of the geoid low / topography high combination, we compute, in a first step, the effects of density anomalies with the shape of a vertical cylinder of a given radius and depth range. With a density anomaly of -1% (corresponding to about 300 K excess temperature) we find that a geoid low of the right size and magnitude can be explained with a cylinder radius of about 10° of arc and the base of the cylinder in the lower transition zone or even lower mantle; with a shallower base the amplitude is under-predicted. On the other hand, if in this case the top of the cylinder is shallower than 150 km, dynamic topography amplitude is over-predicted. The fact that the residual topography high (more sensitive to density anomalies at shallower depth) is laterally displaced relative to the geoid low (more sensitive to greater depths) could indicate a plume or upwelling that is tilted due to large-scale flow. In order to test this possibility we run models with the Aspect mantle convection code of a plume that enters at the base of a box corresponding to a 3300 km x 3300 km region in the upper mantle. However, these plume models have typically a narrow conduit (much narrower than  $10^{\circ}$  of arc) and the plume tends to only become wider as it spreads beneath the lithosphere, i.e. reaching depths of 50 km, hence it would tend to rather over-predict topography and under-predict the geoid.



Figure: Geoid (corrected for crust, and ocean floor age) with respect to equilibrium shape, and residual topography (observed topography corrected for crustal thickness and ocean floor age). The right panel shows geoid (blue) and residual topography (red) along the profiles in the left and center panels.

## Asthenospheric flow estimates in the Atlantic realm based on Poiseuille/Couette flow models

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Mantle convection has profound effects on the Earth's surface, such as inducing vertical motion, which is commonly termed dynamic topography. Sophisticated mantle convection models have been used to study current and past dynamic topography. But many input parameters, like complex rheologies and thermo- chemical flow properties remain poorly known, requiring ad-hoc model parameterization and long-range extrapolation. This makes it attractive to explore simple analytic models of upper mantle flow. The existence of a weak asthenosphere allows one to explore upper mantle in the context of Poiseuille/Couette flow. The latter provides a geodynamically plausible link between flow properties and dynamic topography. Here we construct simple upper mantle flow models parameterized in terms of sources/sinks (plumes/slab) of Poiseuille/Couette flow. Our approach provides physical insight into the pattern of upper mantle flow, makes it easy to assess uncertainties of key model parameters, such as poorly resolved asthenospheric thickness and viscosity, and can be extended back in time, given first--order estimates of plume and subduction flux deduced from geological records. Importantly, it demands low computational cost relative to a time dependent geodynamic models. We present results for the Atlantic realm, and link our estimates of upper mantle flow history to Base Hiatus Surfaces (BHS). The latter serve as proxy for inferring past dynamic topography variations. We also relate our calculations to seismically inferred anisotropy, as a further proxy for upper mantle flow. Our results indicate that asthenospheric flow pattern can be explained through the concept of source to sink and that this flow type is testable against first-order seismic and geologic observables.



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## Geophysical Biogeography

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Attempts to understand the present-day patterns of biodiversity often seek to relate them to the current environmental conditions. However, the present-day distribution of species is only a snapshot of a process that must be seen in geological time. This distribution results from the interaction of biotic and abiotic factors at time scales that range from the instantaneous to the time of the earliest appearance of life on Earth. Of course, while the current knowledge of species distribution at the surface of the Earth is already patchy, the accessibility of data over geological time even more significantly challenges the biogeographer on their quest. The fossil record gets sparser and sparser as we venture in the far past of the Earth, all the way back to Australia's 2.7 Ga Pilbara sediments, where the earliest indications of prokaryotes have been found.

To start with, a theater needs a stage, and the physical conditions need to be set. Zooming out, we are left with few physical inducements to invoke: only geology and climate can set the environmental conditions and prompt the development of a biosphere. Australia has kangaroos, South America has anteaters and Madagascar has lemurs; these charismatic endemics readily attest to the long-term environmental isolation of their native lands. Likewise, extinct species, such as mammoths and saber-toothed tigers, witnessed rapid climate changes. Time and space scales are crucial to linking physical geography and evolutionary forces. Unraveling these relationships would be facilitated if the characteristic time and space scales were unique and constant, but the challenge is to unravel their consequences on the biota, in light of their tempos. Rapid changes can overprint the slow pace of continental drift. Mass extinctions are good examples, where massive and swift changes in geophysical conditions - both climatic and geological - lead to the brutal collapse of numerous species. The current mass extinction of the biosphere has a subtler pathway: humans first modified the physical environment to an extent and pace unrivaled in geological time, and it is only as a feedback relationship that this disruption has led to the current erosion of biodiversity. Deciphering the physical causes of evolution of the biosphere as we know it today, as well as in the past, from the phylogenetic and fossil archive, within the not-so-serene geological history, is the overarching objective of *geophysical biogeography*.

During this lecture, we will review the underlying concepts and processes at play, and illustrate them with a range of pleasant and hopefully inspiring case studies.



# Long term tectonic modelling: specifities, issues and open questions

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One of the main specificity of long term tectonics modelling is that you often needs to apply it to a specific region to validate your model. It ends up being a delicate exercise that involves walking a tightrope between geologists that often find your models too simple and modellers who find it too intricate. While the modelling communities debate on the validity of the boundary conditions and the many parametrization used in our models, geologist will debate about initial conditions. This is sometimes hard to navigate and this causes some mistrust in the validity or usefulness of models.

In this presentation, I will present recurrent debates that are intrinsic to the nature of the problem paused. This includes two debates which I will focus on : the usefulness/validity of fully dynamic and kinematic driven simulations at regional scale and the treatment of pre-existing heterogeneity and flaws, so called inheritance.

I will illustrate these questions with recent studies at different length scales, including subduction driven continental break-up, long term rifting models, accretionary wedge formation and subduction interface rheology. All these problems share debatable initial and boundary conditions. The subduction driven continental break up illustrate the issue of initial conditions (how to start a subduction if you are not interested in modeling that problem) and the use of kinematic boundary conditions and their larger scale meaning. Long term rifting models opens also the debates about forces versus kinematics as boundary conditions. Going to smaller scale, I will tackle the issue of thermal boundary conditions through both continental rifting and accretionary prism dynamic example (see figure). Finally I will go down scale again and discuss boundary conditions and treatment of inheritance issues at the scale of shear zones.

These examples will help me to draw a picture of questions that it would be desirable to address as a community in order to build or rebuild the trust of other communities in the result and usefulness of numerical simulations of long term tectonic processes and to ensure that the community of users makes good use of the tools that are becoming more widely available.



Comparison between temperature (top) and heat flux (bottom) boundary conditions on the dynamic of a simple accretionary prism model.

## Constitutive laws for the brittle lithosphere: Insights from structural geology and experimental rock mechanics

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Fracturing and faulting play a crucial role in shaping the boundaries of tectonic plates. Adequate representations of brittle deformation are thus essential ingredients of long-term tectonic simulations. Modeling the initiation and evolution of faults specifically requires an activation threshold for irreversible strain, and an inelastic flow rule that captures the dynamics, characteristic time scales and macroscopic expression of the underlying grain-scale deformation mechanisms. This is commonly achieved with rate-independent Mohr-Coulomb plasticity coupled with strain softening of cohesion and/or friction. This framework captures fundamental properties of brittle deformation such as a strong dependence on confining pressure, and the possibility of spontaneous localization. It however has potentially important shortcomings, which we seek to remedy by leveraging insight from structural geology and experimental rock mechanics.

First, the standard approach strongly depends on ad-hoc softening parameters such as the characteristic plastic strain over which strength is lost. These often lack a clear mechanistic interpretation, and cannot be determined experimentally. We argue that these parameters may instead be constrained by exploiting the pattern of diffuse brittle strain developing around major faults in tectonic simulations. To this end, we present a workflow aimed at predicting the geometry and orientation of finite brittle strain due to slip on small (sub-grid) mode-I and mode-II fractures, which can be compared to field observations of outcrop-scale faults and fractures, in order to calibrate softening parameters.

The second limitation of the standard approach is that it fails to capture important properties of rocks documented in brittle deformation experiments. These include permanent weakening of elastic moduli prior to macroscopic failure, and the ability of rocks to creep when subjected to stresses below their peak strength. To include them in tectonic simulations, we develop a new constitutive law inspired by damage mechanics and empirical laws of sub-critical fracture growth. In our Sub-Critically-Altered Maxwell (SCAM) flow law, the growth of damage represents the lengthening of tensile cracks around frictionally-activated shear defects. It progressively and permanently weakens the rock's elastic moduli, and accounts for an effective brittle creep viscosity, while determining the onset of localization based on a crack coalescence threshold. The associated micro-mechanical parameters can be fully calibrated against deformation experiments conducted under constant strain rate and constant stress. The SCAM flow law can produce Coulomb-oriented shear bands that initiate as damage bands, and allows a straightforward connection to standard plasticity for large strains. It also enables investigations of parameter upscaling, from grain to lithosphere.

Overall, this presentation will highlight the need for pluri-disciplinary approaches in assembling a constitutive law for the brittle lithosphere. It will also open perspectives for the parameterization

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of tectonic inheritance, and the strain rate dependence of upper crustal deformation.

Figure: **A.** Accumulation and localization of brittle damage in a rock sample [Crider, 2015]. **B.** Sample-scale damage growth and banding in a numerical model based on the SCAM framework.

★ Invited speaker

## 3D lithospheric strength contrast controls on far-field and syntaxial orogens: inferences from the Himalayas and comparison with model results

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The partitioning of the convergence between two continental plates into subduction and shortening is determined by the degree to which compressional stresses are transferred into the lithosphere and strain localises. Strain localization is controlled by rheological contrasts, material parameters, surface processes, and convergence rate (e.g. Vogt et al., 2018). Far-field orogenesis is the geological term used to describe the localization of deformation and formation of an orogen far away  $(10^2)$ -  $10^3$  km) from the collision front. Recently, geological observations have indicated that the thrust faulting along the northern side of the Tibetan Plateau is of similar age as the onset of the remarkably fast continental collision between India and Eurasia. Recent 2D numerical geodynamic modelling suggests that the occurrence of across-strike lithospheric strength variations determine whether a far-field orogen forms (Huangfu et al., 2022). However, the India-Eurasia collision zone is a highly complex area with along-strike as well as across-strike lithospheric strength differences. Here, we investigate the localisation of strain in a corner collision setting based on the Eastern corner of the India-Eurasia collision zone. To this end we use I3ELVIS (a three-dimensional geodynamic code using finite-difference, marker-in cell techniques, with viscoplastic rheologies Gerya and Yuen, 2007), to run 3D coupled lithospheric models with laterally varying boundary conditions. The geodynamic model is coupled to FDSPM, an advection-diffusion-based surface process model (Munch et al., 2022). The simulations are carried out on a 1000 x 1000 x 200 km domain with a uniform grid spacing of 2 km. We vary the rheological contrast through the Moho temperature of the Eurasian domain. We discuss the results of several models (e.g. Fig. 1) which depict distinct scenarios of strain localisation and orogen/plateau formation and compare the results to nature. The initial configuration of inherited rheological heterogeneities, such as suture zones, and convergence azimuth influence where an orogen forms.



Figure 1: Strain rate invariant field overlain by 1 km topography and temperature contours (400°C, 600°C and 1200°C) and surface velocity arrows for the model with a  $T_{Moho}$  contrast of 200°C.

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## Geodynamic modelling of the Wilson-cycle: towards a better understanding of the role of accretionary inheritance

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The Wilson Cycle of closing and opening of oceans is often schematically portrayed with 'empty' oceanic basins. However, bathymetric and geophysical observations outline anomalous topographic features on the seafloor, such as microcontinents and oceanic plateaus, that can be accreted when oceans close in subduction. This implies that Wilson Cycle rifted margins have formed in regions characterized by the presence of previously accreted terranes. The main factors controlling where and how such continental rifts localize in relation to the inherited compressional structures is yet to be explored properly.

We use 2D finite-element thermo-mechanical model experiments to investigate how the number and size of accreted microcontinents as well as the size of the collisional orogen affect the style of continental rifting. We focus on the degree of reactivation of inherited compressional structures: the subduction interface, orogenic thrusts and the thickened crust of the orogen. The subduction interface and thrusts have low brittle strength in our models because of imposed strain-weakening whereas the thick crust of the orogen is weak in a ductile sense because of increased radiogenic heat production.

We find that rifted margins resulting from the extension of an orogen tend to be wide and asymmetric, regardless of the involvement of accretionary terranes. This agrees with earlier numerical studies that show how a weak continental lower crust favours the formation of a wide, asymmetric rift. However, the degree of reactivation of compressional structures – especially the subduction interface – changes with the presence of accreted microcontinents as well as with the size of the orogen and the length of a quiescent period between orogeny and rift-initiation. Narrow orogens that involve no terrane-accretion produce narrow rifted margins on the side of the overriding plate with prominent reactivation of the subduction interface. The length of the quiescent period between orogeny and the onset of rifting has only a second order effect.

In contrast, wide orogens – with or without terrane accretion – localize rifting away from the subduction interface. In these experiments the subduction interface is temporarily reactivated but deformation quickly shifts to the thick orogenic assembly with prominent ductile deformation in the lower continental crust promoting localization of simultaneously active conjugate shear-zone pairs in the brittle crust above. Rifting in these experiments occurs within the subducting plate with varying amounts of crustal material changing affinity from the incoming continent to the overriding continent. These experiments produce very asymmetric margins with an ultra-wide margin on one side.

Our results demonstrate the wide range of features that can form in the presence of inherited compressional structures and emphasise the importance of taking the deformation history into account when trying to understand the evolution of continental rifting.

## Geodynamic and seismological modelling of the Central-Western Mediterranean Cenozoic evolution and present-day structure.

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The Central-Western Mediterranean (CWM) is one of the most complex tectonic setting on Earth. Episodes of slab rollback, break-off and tearing, the opening of back-arc extensional basins (i.e., Liguro-Provencal, Alborean, Algerian and Tyrrhenian basins), the presence of large mountain ranges, active volcanoes and violent earthquakes have made the Mediterranean an ideal environment to study a wide range of geodynamic processes and an important target for seismological studies (e.g, seismic tomography). Here we build a geodynamic model which, although it does not reproduce its exact tectonic structure (e.g., due to the limits of the numerical method, approximations in the initial setup, etc), presents multiple and geometrically complex subduction systems analogous to those found in the CWM. The tectonic evolution of this model is estimated with petrological- thermo-mechanical 3D simulations, then, we dynamically compute the upper mantle fabrics and seismic anisotropy as a function of the strain history and local P-T conditions. After comparing the model with SKS splitting observations in order to quantify the discrepancies with the true Central-Western Mediterranean, we use the elastic tensors predicted for the modeled configuration to perform 3D P-wave anisotropic tomography by inverting synthetic P-wave delay times. Using the geodynamic model as reference, we evaluate the capabilities of a recently developed seismic tomography technique to recover the isotropic anomalies and anisotropy patterns related to a complex subduction environment in different conditions, such as poor data coverage and bad data quality. We observe that, although P-wave tomography still remains a powerful tool to investigate the upper mantle, the reliability of the retrieved structures strongly depends on data quality and data density. Furthermore, the recovered anisotropic patterns are consistent with those of the target model, but in general an underestimation of the anisotropy magnitude in the upper mantle is observed. In the light of future developments, our study suggests that by combining micro- and macro-scale geodynamic simulations and seismological modeling of seismic anisotropy it will be possible to reproduce, at least to a first order, the tectonic evolution of real study regions (e.g., the Mediterranean) thus providing fundamental constraints on the processes that have contributed in shaping their current geological scenario.



Left: final stage of a K) geodynamic model of Central-Western Mediterranean. The plates are highlighted by the Present-day blue surfaces indicating cold material. Purple material at the surface is continental crust.

Right: synthetic anisotropic 30 Ma P-wave seismic tomography of the study area. The color scale indicates isotropic P-wave anomaly, while the black bars the orientation of the fast P-wave axis. The major axis of ellipses is proportional to anisotropy magnitude, while the short axis to the dip of the fast axis. From Lo Bue R, Rappisi F, Vanderbeek BP and Faccenda M (2022) Tomographic Image Interpretation and Central- Western Mediterranean-Like Upper Mantle Dynamics From Coupled Seismological and Geodynamic Modeling Approach. Front. Earth Sci. 10:884100. doi: 10.3389/feart.2022.884100

## The formation of migmatite domes by convection and diapirism in partially molten crust

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Crustal roots from the Archaean to the Phanerozoic arrive to the Earth's surface sometimes in domed structures of kilometer to deca-kilometer sizes. Also called migmatites domes, they attest of the dynamics of partially molten crusts and associated heterogeneous mass redistribution. We model here numerically the development of gravity instabilities in a continental crust heated from below with no lateral motion, simulating the conditions prevailing at the transition between orogenic convergence and collapse. Basal heating is applied for 20 Ma below a felsic crust of 45 km thick. The chemical and physical heterogeneity of the medium is represented by deformable inclusions of distinct viscosity and density with power-law temperature and strain-rate dependent viscosities. We use the VOF Method (Volume Of Fluid, OpenFoam code) that reproduces well the coalescence and separation of inclusions, of sizes a few hundred meters.

In previous work (Louis-Napoleon et al., GJI, 2021) we identified three flow regimes depending on two Rayleigh numbers RaUM and RaPM, for the solid and molten domains, respectively. A "supension" regime describes the entrainment of the heterogeneities in the convective cells, a "layering" regime characterizes how the buoyant inclusions gather as buoyant clusters under the rigid upper crust. A third "diapirism" regime occurs, without convection.

Here we present 2D and 3D models that target the formation of kilometer scale dome structures in the "suspension" and "layering" regimes, to compare with the ca. 5 km size domes of Naxos Island (Greece). These rocks record several cycles of zircon precipitation dated from 24 to 16 Ma, indicating convective motion (Vanderhaeghe et al., 2018). We display several configurations in which the viscosity and density distributions, and basal heating were varied. We discuss the conditions for which domes of partially molten felsic rocks of sizes ca. 5 km form and stagnate at ca. 15 km depth. The role of the size and concentration of the inclusions pinpoints the basic properties of the crust's heterogeneity upon melting.
# Geodynamic modelling of a strike-slip fault with a restraining and releasing bend including surface processes

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We present 3D numerical models of a strike-slip fault including a restraining and a releasing bend. The models are computed with the geodynamic code ASPECT with has recently been two-way coupled to the surface evolution code FastScape enabling us to study the interplay of surface processes and geodynamics in a single framework. At the releasing bend, we observe that sedimentation fosters longer growth and lifetime of the pull-apart basin. At the restraining bend, surface processes are responsible for the concentration of slip onto a few number of faults. These show strain partitioning with the central fault being in a strike-slip regime while the outer faults are reversely faulting which is not observed in the purely geodynamic comparison model. Contrary, the surface traces of the fault network only show minor influence of the surface processes efficiency but are a result of the localization phase. Another key observation is the evolution of many highly asymmetric features despite symmetric initial and boundary conditions. The Dead Sea Transform is a natural example for a continental strike-slip fault with restraining and releasing bend. Despite the generic nature of our models, we can fit many observables such as the depth, asymmetry, and heat flow of the Dead Sea Basin or the differences in surface elevations between the Lebanese restraining bend and the surrounding landscape.



Figure 1: Model evolution of the coupled 3D strike-slip setup with restraining and releasing bend. Upper panel: topography, sediment thickness and mein rivers. Lower panel: vertical velocity as colour scale, surface velocity field as arrows, strain rate in grey to black.

# Hydro-mechanical modelling of seismic cycles in a poro-viscoelasto-plastic fault structure

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A central goal in earthquake physics is to develop a framework that couples solid rock deformation and fluid flow to better understand the role of fluids in seismic and aseismic deformation in natural fault zones. In this context, the aim of this study is to present a newly developed, Hydro-Mechanical Earthquake Cycle (H-MEC) numerical code, which can resolve inertia- and fluid-driven seismic events to simulate fluid-driven earthquake cycles on a fluid-bearing fault structure.

The continuum based, two-dimensional (2-D) code uses a staggered-finite differences marker-incell method (SFD-MIC) to solve the mass and momentum conservation equations for solid matrix and fluid coupled to a poro-visco-elasto-plastic compressible medium. The brittle/plastic deformation is resolved through a rate- and fluid pressure-dependent strength formulation. Global Picard-iterations and an adaptive time stepping algorithm are incorporated to accurately resolve both long-term deformation and short-time earthquake source processes, ranging from years during slow tectonic loading to milliseconds during the propagation of dynamic ruptures.

We present a 2-D in-plane strike-slip fault setup in which we investigate the influence of the poroelastic (de)compaction and hydraulic properties on the occurrence of seismic and aseismic slip. Our modelling results indicate that the nucleation of seismic events is controlled by the viscoplastic compaction of pores and the self-pressurization of fluids inside the fault zone, whereas the propagation of dynamic rupture is driven by solitary pore-pressure waves. Based on our results, permeability and compaction viscosity can highly influence the recurrence interval of seismic cycles as well as the slip velocity of earthquakes. Moreover, changes in permeability and porosity can control the sequences of seismic and aseismic slip behavior on the fault zone.

With this new numerical framework, we can better understand fluid-driven seismicity, and the effects of fluids on long-term geodynamic processes. Furthermore, this methodology can also be applied to model seismic cycles along different tectonic settings, and it allows us to explore seismicity and geodynamic processes within a single numerical framework.

# Sea level and dynamic topography change since the Pliocene: Leveraging a global dataset of twelve wavecut scarps

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Earth's global mean sea level (GMSL) in the past provides a measure of ancient ice volumes. Sea level during the Pliocene in particular, when CO2 and temperatures were above those of the present day, was significantly higher as a result of reduced global ice sheet coverage. Given the similarity of near-future (<100 years) climate to that of the Pliocene, constraining sea level and inferring ice sheet sensitivity during this interval can improve calibrations of predictive ice sheet and sea level models. Unlike proxy-based approaches, geologic deposits directly record past local sea level. However, glacial isostatic adjustment (GIA) and mantle dynamic topography (DT) deform their elevations and cause local sea level to diverge from the global mean. Numerical predictions of deformation caused by both of these processes are necessary to infer GMSL but are highly sensitive to small changes in parameters, hindering their ability to be used as corrections. To address this challenge, we exploit a global dataset of 12 wavecut scarps that formed in the Pliocene, as well as auxiliary geodynamic observations, to improve parameterization of mantle convection models, forward predict solid Earth deformation over the last 3 – 5 Myrs, and compute GMSL in the Pliocene.

To model DT change since the Pliocene, we back-advect the present-day 3-D buoyancy structure of the mantle and calculate the difference in radial surface stresses over the last 3 – 5 Myrs using the convection code ASPECT. We include a wide range of present-day mantle structures constrained by seismic tomography models, including SL2013sv and GLAD-M25 in the upper mantle and TX2011, S40RTS, S362ANI+M, and GLAD-M25 in the lower mantle. Above the 410-km discontinuity, we convert seismic wave speeds to temperatures using a laboratory-based conversion scheme that accounts for the effects of anelastic deformation and is calibrated with independent geophysical observations. In the lower mantle seismic velocities are converted to temperature with a simple anharmonic approach, as the effects of anelasticity are less dominant. We further implement 3-D viscosity models that are consistent with the computed present-day mantle temperatures. By leveraging the differential elevations of each scarp, we identify the simulations that best reproduce the observed deformation, and we use these models as well as predictions of GIA to estimate GMSL across the Pliocene.

# Controls on plate tectonic evolution

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The operation of plate tectonics has moulded our planet's surface and influenced the deep interior. Despite its significance, the inception of plate tectonics and its subsequent evolution are still heavily debated. Recent studies have suggested that since 3Ga the rise of the continents and accumulation of sediments at continental edges and in trenches has provided lubrication for the stabilization of subduction and therefore is a crucial factor in controlling plate tectonic evolution (Sobolev and Brown, 2019 Nature). In order to test this hypothesis, we aim to build efficient 3D mantle convection models coupled with surface processes. As a first step towards reaching this aim we present compressible 2D visco-plastic global mantle convection models with 100My-old lithosphere, a composite rheology and realistic phase transitions using the open-source geodynamic modelling code ASPECT. Through the use of adaptive mesh refinement, we are able to reach high resolution in localized features such as trenches or at the free surface. We then present models with various so-called mobility-friction functions. Specifically, in a given range, as mobility (surface velocity/mantle velocity; the extent to which the lithosphere is able to move in a given time frame, when compared to the mantle) increases friction is decreased to emulate an increase in delivery of sediments to trenches. This reduction in friction leads to more subduction zones. The correlation between mobility and friction is not clear however we do find instances where decreasing friction correlates with increasing RMS velocity. These predictions correlate well with observations from paleomagnetic reconstructions in the Phanerozoic/Neoproterozoic which also show an increase in RMS velocity of around 10cm/yr after the snowball earth glaciation event. RMS velocity then decreases from 15cm/yr back to 5cm/yr over a 300Ma time span. We have begun to expand on these simplified scenarios by including stable continental lithosphere, which will likely lead to a better fit with observed plate velocities. Moreover, we have begun expanding into 3D whereby the role of plumes on plate tectonics is expected to differ greatly.

# The effect of permeability on the pressure regime in 2D outcropto-outcrop submarine hydrothermal flow models

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The significant discrepancy between the observed conductive heat flow and predictions by thermal models for oceanic lithosphere younger than 50 Ma is generally interpreted to result from hydrothermal circulation between basement outcrops. Numerical simulations of fluid flow between such outcrops performed in previous studies revealed that establishing horizontal pressure gradients to sustain a hydrothermal siphon requires high aquifer permeabilities and a contrast in the outcrops' transmittance, which is the product of the outcrop permeability and the area of outcrop exposure. However, most previous studies focused on the model parameters needed to sustain a hydrothermal siphon, while the physical processes that create the horizontal pressure gradients in the first place remain poorly constrained.

In order to shed more light on the physics behind outcrop-to-outcrop flow, a simple synthetic 2D model of two outcrops connected by a permeable aquifer was set up. Fluid flow modelling was done by using hydrothermalFoam, a hydrothermal transport model, that is based on the opensource C++ computational fluid dynamics toolbox OpenFOAM. Our initial simulations focus on variations of the permeability of the outcrops and the aquifer. The results reveal two key points that are essential to generate a flow: First, the outcrops permeability has a fundamental effect on its average pressure. High permeabilities lead to a rather "cold" hydrostatic pressure regime with lower temperatures and hence higher average pressure. Lower outcrop permeabilities are accompanied with a rather "warm" hydrostatic pressure regime characterized by higher temperatures and lower average pressures. Secondly, fluid convection in the aquifer is necessary to establish a siphon flow. Therefore, the aquifer permeability must be sufficiently high to overcome Darcy resistance and yet low enough to prevent the flow from being solely diffusive. Since the occurrence of outcrop-to-outcrop flow is reflected by gradients of the conductive heat flux in the overlying sediment layer, heat flow measurements on the seafloor may not just help to indicate a hydrothermal siphon but may also contribute to constraining the permeability structure of the basaltic crust.

# Present-day upper-mantle architecture of the Alps: insights from data-driven dynamic modelling

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The dynamics of the Alps and surrounding regions is still not completely understood, partly because of a non-unique interpretation of its upper-mantle architecture. In this respect, it is unclear if interpreted slabs are consistent with the observed surface deformation and topography. We derive three-end-member scenarios of lithospheric thickness and slab geometries by clustering available shear-wave tomography models into a statistical ensemble. We use these scenarios as input for geodynamic simulations and compare modelled topography, surface velocities and mantle flow to observations. We found that a slab detached beneath the Alps, but attached beneath the Northern Apennines captures first-order patterns in topography and vertical surface velocities and can provide a causative explanation for the observed seismicity.



Mean-std model 220 km Mantle FlowMean model 220 km Mantle FlowMean+std model 220 km Mantle FlowModelled topography for a) mean-std, b) mean, and c) mean+std models. Earthquakes from the<br/>AlpArray Research- Seismicity-Catalogue (Bagagli et al., 2022) are plotted with circles<br/>color-coded by depth: orange 0-20 km, red 20-40, km, and blue > 40 km and scaled by the<br/>magnitude (Mc = 2.4). Modelled Vertical velocities at 10 km depth for d) mean-std, e) mean, and<br/>f) mean+std models with GNSS measurements plotted in circle (Sternai et al., 2019). Horizontal<br/>flow in the asthenosphere at a depth of 220 km for g) mean-std, h) mean, and i) mean+std models<br/>are plotted as green lines scaled by velocity magnitude. SKS splitting measurements scaled<br/>according to the delay time are plotted with black bars (Hein et al., 2021). White lines in these<br/>last three panels indicate the contour of the slabs.

# From orogeny to rifting: the role of inherited structures during the formation of the South China Sea

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Continental rifts often form in places where lithospheric weaknesses are inherited from previous orogenic events. How structural, compositional, and thermal inheritance controls the inception and evolution of rifting, as well as the final architecture of rifted continental margins remains unclear. Here we focus on the South China Sea, which experienced tectonic inversion from a Mesozoic Andean-type orogeny (i.e., Yanshanian orogen) to a Cenozoic rifted continental margins. Recent acquisition and interpretation of seismic profiles, drill cores, and geochronological analysis allowed for the identification of Mesozoic strata, magmatic rocks related to a former arc and pre-Cenozoic fault systems in the South China Sea. It appears that the pre-rift lithosphere is not homogeneous, so our multi-stage models allow us to illustrate the impact of inheritance on rifted margin spatiotemporal evolution and the final architecture.

Here, we employ a numerical forward model that includes a two-way coupling strategy (Neuharth et al., 2022) linking the geodynamic code ASPECT (Kronbichler et al. 2012; Heister et al. 2017) and the landscape evolution model FastScape (Braun & Willet, 2013; Yuan et al., 2019). We reproduce the first-order kinematic evolution of the South China Sea by imposing a phase of continental collision, followed by tectonic quiescence and extension. We quantitatively evaluate a suite of models that vary the convergence velocity, heat production, and erosion rate.

The reference model reproduces a range of tectonic regimes including continental collision, postorogenic collapse, continental rifting and lithospheric breakup. Our results show that crustal rheology and temperatures exert a primary control on the occurrence of either a double-vergent orogen or an asymmetric orogen with continental subduction. Further, we find that not all inherited thrust faults are reactivated when the orogen collapses. However, faults reactivated during subsequent extension are important in controlling strain localization during the early stages of rifting. In our models, however, inherited structures related to the mechanical weaknesses in continental crust do not significantly control the location of breakup and the rifted margin architecture. We propose that decoupling between deformation within the crust and mantle, as is typically inferred for wide rifts like the South China Sea, reduces the impact of crustal-scale inheritance. Rifted margin formation is instead dominated by newly-formed extensional shear zones. We suggest that this finding is applicable to other wide rifts worldwide, such as the Basin and Range Province, the Aegean Sea and the West Anatolian extensional system.

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# Numerical modeling of the lithospheric structural control on the deep carbon transfer during intracontinental extension

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Continental rifts are essential sources of deeply derived CO2 emission into Earth's atmosphere since faults act as permeable pathways for the ascent of the CO2. As the largest active continental rift, the Eastern African Rift (EAR) shows distinct variation in carbon flux and sources between the Archean craton (a low crust-deriving CO2 flux) in the west and the Proterozoic orogen (a high mantle-deriving CO2 flux) in the east. It has been suggested that the Archean craton is a massive carbon reservoir by long-term metasomatism in geological timescales, while the hot orogen is a carbon-lacking zone due to its instability by a large thermal gradient. This distinct feature and underlying mechanisms remain an outstanding question. Here we construct 2D petrological-thermomechanical numerical models to investigate the influence of the lithospheric structures on the deep carbon transfer during continental rifting.

Our preliminary model results show that the deep carbon transfer is primarily controlled by mantle melting and continental rifting. Under extension, a carbon layer with lower density (3200 3300 kg m-3) and low viscosity ( $5.01 \times 10^{16} > \eta_0 > 5.01 \times 10^{20}$  Pa<sup>n</sup> s) tends to transfer upwards, thus emitting more mantle-derived CO2 to the atmosphere through melting and crustal faults. The craton thickness has little influence on the rifting and melting process; however, a higher thickness gradient of the lithosphere step between the craton and the orogen promotes carbon transfer. Rift forms in the middle of the orogen lithosphere despite different crustal thicknesses, Moho temperatures, or extensional rates. Nonetheless, higher Moho temperature and extensional rate can produce more melting and faster rifting, thus encouraging carbon transfer. More detailed investigations regarding the viscosity and density of the carbon layer at the bottom of the lithosphere and factors controlling the melting and rifting processes are needed to explain the mechanism of deep carbon transfer in the EAR.

# Evolution of rift systems and their fault networks in response to surface processes

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From rift initiation to continental breakup, a rift evolves through different stages that produce distinct rifted-margin domains and major sedimentary basins. While the existence of these stages can be inferred from geophysical and geological data, it is not as well understood how the fault network changes throughout these stages. Additionally, different rifts undergo varying amounts of erosion and sediment deposition, which is suggested to influence fault longevity (e.g., Andrés-Martínez et al., 2019) and may affect overall rift evolution. Previous work has qualitatively analyzed the effects surface processes have on rift and fault evolution, however, there has not been a qualitative approach to analyze changes to the fault network over time.

In this study we ran 12 high-resolution 2D rift models utilizing a two-way coupling between the tectonic code ASPECT (Heister et al., 2017) and the landscape evolution code FastScape (Yuan et al., 2019). Using FastScape, we vary the efficiency of surface processes through the bedrock erodibility (Kf) from no sedimentation or deposition to low ( $K_f = 10^{-6} \text{m}^{0.2}/\text{yr}$ ), medium ( $10^{-5} \text{ m}^{0.2}/\text{yr}$ ), and high efficiency ( $10^{-4} \text{ m}^{0.2}/\text{yr}$ ). These different surface process efficiencies are applied to three separate models that represent a symmetric, asymmetric and wide rift. As we are interested in the effects surface processes and rift type have on the fault network, we analyze the models using a novel quantitative fault analysis toolbox (https://github.com/thilowrona/fatbox) that allows us to track and correlate discrete faults through space and time. Utilizing this toolbox, we track the number of faults and the evolution of their properties such as cumulative length and displacement (Fig. 1a-d) to see how these parameters change depending on the rift type and efficiency of erosion and sediment deposition.

By analyzing how the fault network properties change through time, we find that a rift evolves through up to 5 first-order phases: 1) distributed deformation and coalescence, 2) fault system growth, 3) fault system decline and basin-ward localization, 4) rift migration, and 5) continental breakup (Fig. 1). This general progression of phases occurs regardless of the type of rift or the efficiency of surface processes, except for the rift migration phase that occurs only in asymmetric models. Additionally, while we find that surface processes do not exert a major influence on the final rifted margin architecture, they affect the temporal evolution of the fault network by increasing fault longevity leading to rift phase prolongation and a delay in continental breakup.



**Figure 1.** Five phases of the fault network during the evolution of an asymmetric rift model. (a-d) show the cumulative fault properties (displacement, length, number of faults, and fault location) of active faults through time, where red indicates an active left dipping fault and blue an active right dipping fault. (e-i) Model snapshots of the fault network overlain on the model for each fault network phase. Figure from Neuharth et al. (2022)

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# Deep structural signatures and temperature controlled rheological transitions in accretionary wedges; insight from thermomechanical modeling

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Significant analogue and numerical studies on the evolution of accretionary prism have often been applied linear (i.e., depth-independent) viscosity, which represents an oversimplified assumption. Here, we solve for advection-diffusion of heat with imposed constant heat flow at the base of the model domain to allow the temperature to increase with burial. We aim to account for heat conservation or temperature-dependent rheological transitions with a simple setup of one décollement layer. Our results show that a mature brittle-ductile wedge consists of four topographically and structurally distinct domains. Two topographically flat domains are associated with either dehydration reactions along the décollement, or with primarily viscous deformation at the back of the wedge. A domain with topographic slope that follows the critical taper theory corresponds to the brittle frontal toe of the wedge. The fourth domain has a topographic slope steeper than what predicted by the critical taper theory. This steep slope is linked with the brittle-viscous transition in the wedge.

We include more complexity in our simulations to increase the relevance of the models with the Makran accretionary prism. We investigate how the active structures of the Iranian Makran vary laterally, and their tectonic interaction with deep structures (i.e., duplexes and seamounts). By testing the influence of different décollements and seamounts on topography and deep structures, we suggest that the presence of a brittle-ductile transition zone and dehydration processes control the downdip evolution of the tectonic structures and the topographic above the upper plate. The onset of underthrusting is controlled by the brittle-ductile transition. Furthermore, the occurrence of normal-faulting events is mostly controlled by the presence of seamounts, while the weakening of friction associated with dehydration and underplating events have a subordinate effect.

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Figure: **a**. Proposed model for the mature brittle ductile wedge which forms three distinct segments; pure brittle wedge with a rather constant slope predicted by the CTT at the front (blue star), low but non zero topographic slope close to the backstop corresponds to viscous deformation (black star) and, larger topographic slope in between these segments as a result of the brittle ductile transition (red star and yellow rectangle). **b**. Topographic slope versus internal friction for  $\phi_{basal} = 5^{\circ}$ . c. Basal friction versus topographic slope for  $\phi_{int} 10^{\circ}$ ,  $17^{\circ}$  and  $25^{\circ}$ .

# Rift segmentation in continental lithosphere: investigations of the required thermophysical conditions through numerical experiments

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The geologic record of deformation occurring in extensional margins shows a complex picture. Even in case the lithosphere is subjected to a uniform stretching and thinning, the resulting extension is inhomogeneously distributed along the formed rift basins. The factors controlling this phenomena, and rift architecture in general, have been identified in the inheritance of pre-rift conditions, such as pre-existing structures, lateral rheological (Heron et. al, 2019) and/or thermal variations (Manatschal et. al, 2015).

In the frame of the ANTIPODE project, whose aim is the paleo-bathymetry reconstruction of the Ross Sea, we investigate the influence of post-rift thermal transients in controlling thermal subsidence. We implement a set of numerical models, simulating syn-rift phases and post-rift conditions, to use as synthetic analogues of real rift systems. We observe that the formation of "localized" basins with undisturbed sides and a necked lithosphere at the center becomes unlikely using a range of initial thermophysical conditions, time and velocity of rifting. In particular, simulating an extension applied to a lithosphere having a uniform thickness and steady state thermal conditions, it is usually obtained a stretched lithosphere with a uniform thinning - close to the theoretical syn-rift deformation of McKenzie (1978).

Therefore, we investigate what are the physical conditions required to obtain the opening of a series of basins from an initial rift phase. The obtained results suggest that inherited crustal heterogeneities and thermal transient conditions of the lithosphere can favor the opening of different basins under extensional tectonics. To this purpose, we implement several 2-D thermophysical models consisting of a multilayer continental lithosphere, which is extended, by applying different amounts of divergent velocities. We use the open source Underworld2 modelling code (Mansour et. al 2020), which relies on Lagrangian integration point finite element approach (Moresi et. al, 2003) and provides a Python API to construct, run, and visualize the output of geodynamic models.

Preliminary results suggest that uniform extension can be caused by a reduction of viscosity in the lower crust, induced by an initial relatively warm crustal geotherm, at steady state conditions. Both compositional changes and cold thermal conditions, inherited from recent tectonics, favour localized deformation, which eventually evolves in a basin morphology sided by two topographic highs. In addition to inheritance, including more than one rift phase, producing the same average extension of one rift phase, has a significant effect on the morphology of the formed rift basins.

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# Residence time of inertial particles in 3D thermal convection: implications for magma reservoirs.

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The dynamic behaviour of crystals in convecting fluids determines how magma bodies solidify. In particular, it is often important to estimate how long crystals stay in suspension in the host liquid before being deposited at its bottom (or top, for light crystals and bubbles of volatiles). We perform a systematic 3D numerical study of particle-laden Rayleigh-Bénard convection, and derive a robust model for the particle residence time. For Rayleigh numbers higher than 107, inertial particles' trajectories exhibit a monotonic transition from fluid tracer-like to free-fall dynamics, the control parameter being the ratio between particle Stokes velocity and the mean amplitude of the fluid velocity. The average settling rate is proportional to the particle Stokes velocity in both the endmember regimes, but the distribution of residence times differs markedly from one to the other. For lower Rayleigh numbers ( $< 10^7$ ), an interaction between large-scale circulation and particle motion emerges, increasing the settling rates on average. Nevertheless, the mean residence time does not exceed the terminal time, i.e. the settling time from a quiescent fluid, by a factor larger than four. An exception are simulations with only a slightly super-critical Rayleigh number  $(10^4)$ , for which stationary convection develops and some particles become trapped indefinitely. 2D simulations of the same problem overestimate the flow-particle interaction – and hence the residence time – for both high and low Rayleigh numbers, which stresses the importance of using 3D geometries for simulating particle-laden flows. We outline how our model can be used to explain the depth changes of crystal size distribution in sedimentary layers of magmatic intrusions that are thought to have formed via settling of a crystal cargo, and discuss how the micro-structural observations of solidified intrusions can be used to infer the past convective velocity of magma.



Figure 1. Crystal size distribution in suspension and sediment for a simple application: the settling of crystal cargo in a solidifying intrusion. We test three values of the fluid mean velocity  $u_{rms}$ , corresponding to a static magma (black), vigorously convecting magma (orange), and to an intermediate case (blue). Solid lines show the size distribution of particles remaining in suspension at the time t = 40 weeks, at which more than 60% of all the particles have settled in all three cases. Symbols display the size distribution in the currently forming layer of sediment. Triangles represent particles with  $v_t > 2.0u_{rms}$  (stone-like), circles show particles with  $v_t < 0.5u_{rms}$  (dust-like), and crosses mark the transition

# Feedbacks between tectonics and hydrothermal circulation – plausible flow scenarios for the TAG hydrothermal field

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The Earth System appears increasingly interconnected and hydrothermal discharge at back smoker vent sites is not only visually appealing, it also sustains unique ecosystems, generates large polymetallic sulfide deposits, and modulates ocean biogeochemical cycles. At slow spreading ridges, fault zones seem to provide stable preferential fluid pathways resulting in the formation of the ocean's largest sulfide deposits. Yet, how low angle faults organize hydrothermal circulation and how fluid pathways can remain intact for 10s-100s kyr remains poorly understood. These processes can be excellently studied at the TAG hydrothermal mound at 26°N on the Mid-Atlantic Ridge (MAR). The active mound is located on the hanging wall of a detachment fault and has formed through distinct phases of high-temperature fluid discharge lasting 10s to 100s of years throughout at least the last 50,000 years. Yet, the mechanisms that control the episodic behavior, keep the fluid pathways intact, and sustain the observed high heat fluxes of possibly up to 1800 MW remain poorly understood. Previous concepts involved long-distance channelized hightemperature fluid upflow along the detachment but that circulation mode is thermodynamically unfavorable and incompatible with TAG's high discharge fluxes. Here, based on the joint interpretation of hydrothermal flow observations, 3-D flow modeling, and semi-analytical solutions, we show that the TAG system can be explained by episodic magmatic intrusions into the footwall of a highly permeable detachment surface. These intrusions drive episodes of hydrothermal activity with sub-vertical discharge and recharge along the detachment. This kind of flow model probably "requires" the ridge segment to be at a special stage of the life cycle of detachment systems, with possibly renewed magmatic activity and surficial faulting of the hanging wall. Taken together, this revised flow model reconciles problematic aspects of previously inferred circulation patterns and allows to identify the prerequisites for generating substantive seafloor mineral systems.



Figure 1: a) geophysical constraints and b) revised hydrothermal flow model for the TAG hydrothermal field.

# Identifying areas of potential future volcanic activity in Germany for safe long-term storage of high-level radioactive waste

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When looking for a repository for high-level radioactive waste in Germany, areas in which quaternary volcanism occurred or future volcanic activity is expected within the next one million years must be excluded. While regions with Quaternary volcanism are known reasonably well, there are currently no generally accepted methods available for the long-term forecast of future volcanic activity in fields of intraplate, distributed volcanism. However, several geodynamical and petrological indicators that provide information about past and potentially recent or future processes connected to magmatic and geodynamic activity could be used for assessments of future volcanism [1, 2, 3].

Here, we present the first results of our applied method, which may allow a regional differentiation of the likelihood of future volcanic eruptions in Germany. The method consists of a semi-quantitative, multi-criterial approach, combining a variety of indicators including, amongst others, occurrence of volcanic rocks and their ages, seismic observations (e.g. depth of lithosphereasthenosphere boundary or mantle anomalies), ground motions, swarm and deep low frequency earthquakes, neotectonic activity, mantle degassing and geodynamic simulations. In total 30 indicators were defined and ranked according to their presumed relevance for long-term predictions of volcanism, following the results of two expert surveys. Properties of parameters and their weights are used to quantify the individual indicators. Thereby, the parameters are uniformly applied for Germany in order to enable a transparent and equal risk assessment of future volcanic activity in all of the federal states (see Fig. 1).



Fig. 1: Overlay of the 10 highest ranked indicators and their weights for a regional differentiation of the likelihood of future volcanic activity in Germany.

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# Intraplate dynamics in Mongolia: Investigating asthenospheric versus lithospheric constraints on landscape evolution.

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Mongolia sits in the centre of the Asian continent and is far from any plate boundaries (Van der Voo et al., 2015). However, volcanism and intraplate uplift have occurred in the region over the past 100+ Myrs, with no clear cause for the dynamic conditions (Hunt et al., 2012, Sheldrick et al., 2018). The main anomalous uplift is found in the form of the Hangai Dome in central Mongolia, which rises >3000 m (Barry et al., 2003). The volcanism is more widespread, producing small volume lavas in areas across the central and south-eastern regions of the country (Hunt et al., 2012, Sheldrick et al., 2018). Mongolia is also the location of the suturing of the Mongol-Okhotsk Ocean, which occurred 140-120 Ma, predating intraplate volcanism and uplift by at least 20 Ma, with additional uplift during the Mid-Oligocene (Van der Voo et al., 2015, McDannell et al., 2018). Several theories have been expressed to explain the volcanism, including mantle plumes, rifting, and delamination, with the latter of these being of current interest (Barry et al., 2003, Hunt et al., 2012, Sheldrick et al., 2018). This study aims to understand the influences played by the architecture of the lithosphere versus the regional mantle flow within the asthenosphere, on the formation of intraplate uplift and volcanism across Mongolia. Geodynamic models are created using the finite- element code Aspect, with Perplex used to create a reference material model for the study. Plate motion histories going back to 410 Ma are extracted from GPlates to recreate mantle convection and investigate the formation of intraplate volcanism, following the closure of the Mongol-Okhotsk Ocean. The model will also be used to understand the influence of the Pacific and Indian Plate collision on the formation of uplift in the Hangai Dome. Localised models will be created using Worldbuilder to recreate the 3D environment roughly 30-35 Ma to test the local impacts on the formation of dynamic topography in Mongolia, and the formation of the Hangai Dome.

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# Initial results of modelling 3D plate dynamics in the Alpine-Mediterranean area

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Tectonic reconstructions of lithospheric plate motion can be approached by different geological methods. However hypotheses derived from these findings are often not validated in a physically consistent manner. Therefore we employ 3D geodynamic modelling in order to test geological reconstructions.

In this work, 3D thermomechanical forward simulations of the Alpine-Mediterranean area are conducted using the software LaMEM (Kaus et al. (2016)). A viscoelastoplastic rheology and an internal free surface are applied, which means that apart from the internal dynamics also the surface response can be investigated. Kinematic reconstructions of Le Breton et al. (2021) at 35 Ma serve as an initial setup for the simulations. The goal of these simulations is to determine the main driving forces of plate dynamics in this area. This is done by evaluating effects of different model parameters such as the thermal structure and the geometry of the slabs, the viscosity of the mantle and brittle parameters of the crust.

The dynamics of the Alpine-Mediterranean area is dominated by the propagation of different subduction zones. Not only old oceanic crust is subducted but also lithospheric delamination leads to propagation of subduction zones. This be-haviour makes the subduction trenches propagate with different velocities causing complex slab geometries and associated mantle flow.

Our results suggest that subduction dynamics in the Western Mediterranean is mostly independent of Africa's plate motion, whereas the movement of the Adriatic microplate is influenced by both the movement of Africa and the propaga-tion of the surrounding subduction zones. Especially in the Apennines, delamination processes of the lithosphere seem to play a key role in the overall subduction dynamics.

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# Thermomechanical modeling of magmatic intrusion, volcanic deformation and flank stability

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Magmatic intrusion and associated volcanic deformation are traditionally approximated with an expanding point source or cavity in an elastic halfspace. The most commonly used model is the "MOGI source" which predicts surface displacement as a function of pressure or volume change, depth and elastic properties of the crust.

Here, we present 3D thermomechanical models that approximate intrusion into a pre-existing magma body with a cylindrical pipe which couples the magma body to a velocity boundary condition at the bottom of the model. The influx of material results in the development of overpressure inside the magma body and subsequent surface deformation.

We show benchmarks, comparing our numerical results for an elastic host rock to the analytical solutions of Mogi (1958) and McTigue (1987). Furthermore, we demonstrate the effects of using a more realistic visco-elastic crustal rheology in comparison to an elastic halfspace. The magnitudes of overpressure and surface deformation change as a function of host rock viscosity and are therefore dependent of the age and thermal structure of the magmatic system.

We also investigate the dynamics of a system that hosts several interconnected magma bodies at different stages of magmatic differentiation. Finally, we show the interplay between the surface deformation and a volcanic edifice and demonstrate how near-surface intrusions can affect the stability of volcanic flanks.

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Results of magma intrusion model. (a) 2D slice through the model after 2000 years. Magma body and feeder zone are outlined in black, arrows indicate established flow field with a parabolic velocity distribution. Background shows overpressure which decays along the feeding system and is homogeneous within the magma body. (b) 10 MPa overpressure contours after 200 years (yellow), 1000 years (blue) and 2000 years (orange). Arrows along the orange contour show velocities that are induced in the crust by the influx of magma. Arrow length shows velocity magnitude and colors indicate vertical component. Axes are in km.

# **Emergence of fault patterns from large-scale continental collision models**

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Mountainous regions featuring an orogenic wedge adjacent to an orogenic plateau are relatively common, but the ways in which these two components co-evolve remain poorly understood. Examples of plateau-foreland pairs include the Himalaya/Tibetan Plateau, the Andes/Altiplano, the Sierra Nevada/Nevadoplano, the Alps/Bavarian Plateau, and the Iranian Plateau to name a few. Understanding the process interactions that drive development and maintenance of the plateau-orogenic wedge system therefore has broad applicability.

On a first-order, this study addresses how orogenic plateaux develop. The plateau-wedge system is hypothesized to evolve as continental collisional systems mature into what is referred to as a "large, hot orogens". The formation of a plateau is hypothesized to be a result of long-term crustal thickening. This results in thermal expansion and the development of excess gravitational potential energy which in turn develops into mid-to-lower crustal channel flow. The primary structural manifestation of the transition between the upper crust and the region of thermally-weakened viscous flow comprising the plateau and surroundings has been suggested to be a regionally extensive decoupling horizon. However, understanding of the development of such structures is limited. Therefore, we generate preliminary models of a lithospheric-scale collisional system that will eventually allow us to investigate what sorts of structures emerge near the transitional region and - by extension - how the plateau-wedge relationship evolves through time.

Here we describe our initial forays into use of the open-source, finite-element geodynamic code ASPECT to explore plateau-wedge interactions. Numerical simulations of a compressional system are performed using ASPECT, which is a massively parallelized code that was originally designed to model thermal convection in the mantle but, in recent years has been extended greatly to successfully simulate deformation of the lithosphere. Our work builds on these efforts, and a lithospheric-scale model of continental collision is generated and the p ost- processing module fatbox is used to analyze the nature of brittle failure in the context of large, hot orogenic systems.

Work from the first stage in this study is presented: including development of a model that demonstrates the evolution from a small, cold orogenic system consisting of a brittle wedge to a large, hot orogen comprised of a plateau-wedge system. Further, post-process analysis of both spatial and temporal strain localization is used as a proof-of-concept for future studies in which extraction of fault patterns will be used to better understand the nature of regionally extensive decoupling horizons that appear in orogenic systems worldwide.

# Continent-continent collisions in the Paleoproterozoic: exploring the effects of convergence obliquity and temperature on P - T - tpaths

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The starting time and mode of plate tectonics is a fundamental question in geodynamics. It is often thought that the Paleoproterozoic Era acted as a transition period from plume-lid tectonics to modern plate tectonics. Metamorphic rocks from the Paleoproterozoic generally lack record of UHP conditions but indicate higher temperatures, which maybe related to different mode of plate tectonics. However, time poses a unique challenge. Paleoproterozoic rocks that can be accessed easily today have been exhumed as a result of deep levels of erosion. We aim to overcome this issue using pressure-temperature-time (P - T - t) paths extracted from generic continent-continent collision models and to compare them to P - T - t paths from metamorphic minerals. 1.92-1.77 Ga ago, the Svecofennian orogeny formed the majority of the bedrock in southern Finland. It is well studied by number of geological and geophysical means, but physics-based geodynamical models of it are still lacking.

Around 1.84-1.79 Ga ago, the continent of Sarmatia collided into Fennoscandia as a part of the Svecofennian orogeny, forming margin-parallel shear zones in present-day southern Finland (Korja et al., 2006). This continent-continent collision was oblique and forms the basis of our numerical models, which test the impact of obliquity on metamorphism. Comparable metamorphic samples are collected from vicinity of the shear zones in southern Finland.

The models were run using 3D thermo-mechanical, finite element geodynamical modeling software DOUAR (Braun et al., 2008), which uses the PETSc version of the direct matrix equation solver MUMPS and the landscape evolution model FastScape. DOUAR has its disadvantages, such as limited resolution due to memory requirements, but it has demonstrated its capabilities when combining surface dynamics with lithospheric dynamics (Nettesheim et al., 2018) to model rock exhumation, for example.

Ongoing work is exploring the effects of various continental collision obliquity angles and temperature conditions in a set of nine different models. The spatial dimensions of the models are  $1000 \times 1000 \times 70$  km and the element size is  $7.8125 \times 7.8125 \times 3.90625$  km. In the Svecofennian orogeny, continent-continent collision was an event between colder and hotter continental blocks, which is implemented in the models by having a temperature difference of  $100^{\circ}$ C on the model base at 70 km. Along this boundary, heat production is varied laterally in three different temperature scenarios. Conver- gence obliquity angle is varied between  $0^{\circ}$ ,  $30^{\circ}$  and  $60^{\circ}$ , while subduction dip angle is  $30^{\circ}$ .



## t=0.7 Ma

Figure 1. Early state of a model with an obliquity angle 30° in the high temperature scenario. Isotherms correspond to temperatures starting at 200°C with a 200°C contour interval.

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# (Exo)planet interior-atmosphere coupling

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One of the main factors to assess the possible habitability of a rocky planet (either in or beyond our solar system) is its capability to maintain an atmosphere that allows for moderate temperatures at the surface and would allow water to occur in a liquid form, and that can help shield surface life from harmful radiation.

The existence of an atmosphere, however, depends on several key factors - possible accretion from the solar nebular, catastrophic degassing from the crystallizing magma ocean during planet formation, later delivery of volatiles via comets, sinks of atmosphere gases to the surface or to space by atmospheric erosion, and last, but definitely not least, volcanic release of volatiles from the mantle that where stored in the planet's interior during its formation stage.

Here I will review important planetary factors (such as planet mass or mantle redox state) that have already been identified to impact the atmospheric evolution of rocky planets (from Earth to exoplanets), and show new investigations on the influence of plate tectonics on the composition of an evolving secondary atmosphere.

# InSights into the interior of Mars: new discoveries and modeling

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Geophysical measurements of the InSight mission [1] were recently used to provide the first detailed look into the Martian interior. The analysis of seismic events recorded by InSight revealed that the radius of the Martian core is at the upper end of previous estimates derived from gravity field measurements. This implies a large amount of light elements such as sulfur, oxygen, carbon and perhaps even hydrogen that in turn provides constraints on the evolution of the core and suggests a liquid state at present day [2]. Marsquakes were also used to constrain the structure of the upper mantle down to 800 km depth, indicating that Mars possesses today a much thicker thermal lithosphere than the Earth [3]. Estimates of the crustal thickness of Mars that have been derived from gravity and topography data have been improved by seismic measurements that provide an anchor point at the InSight landing site. The seismic measurements combined with gravity and topography data indicate that the crust is thinner and lighter than previously suggested [4].

We will present an overview of the InSight results on the Martian core, upper mantle structure, and crust, and discuss how the InSight data and additional constraints from tidal deformation, elastic lithosphere thickness, and prolonged volcanic activity can be used together with geodynamical models to investigate the thermal evolution of Mars [5]. Results from geodynamical thermal evolution simulations that include the effects of the most recent crustal thickness models show that crustal thickness variations (Fig. 1a) control the lithospheric temperature variations and thus affect the lithospheric seismic velocities (Fig. 1b), surface heat flow (Fig. 1c), the elastic lithosphere thickness (Fig. 1d), and the location of partial melt zones in the present-day Martian mantle (Fig. 1e). The crustal and thermal lithosphere thickness estimates from InSight suggest that the Martian crust stores more than half of the planet's total amount of heat producing elements. The large size of the Martian core leads to a smaller scale convection pattern in the mantle than previously suggested. Models show strong mantle plumes that produce melt up to recent times in Tharsis and Elysium, while weaker plumes are distributed throughout the mantle. The thickness of the seismogenic layer, where seismic events can occur, shows a variability that correlates with the crustal thickness (Fig. 1f). Furthermore, model predictions of present-day Martian seismicity can be compared to the values measured by InSight in order to select successful models.



Fig. 1: Geodynamical modeling of the interior of Mars: a) crustal thickness model derived from gravity and topography data and anchored by the crustal thickness at InSight location; b) corresponding shear wave velocity variations at 400 km depth; c) surface heat flow; d) elastic lithosphere thickness variations; d) average melt fraction; f) seismogenic layer thickness computed using the 573 K isotherm. All maps show values calculated at present day.

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# **Regional-Scale Lithospheric Recycling on Venus via Peel-Back Delamination**

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The tectonic forces that have shaped Venus' surface over time are currently not well understood. Over 10,000 km of possible subduction sites have been identified on Venus, many of which are located near groupings of rift-zone trenches called chasmata [1]. Until now, no studies have tested the viability of subduction initiation at a rift zone on Venus. Here, we created 2D numerical models to determine if and how regional-scale lithospheric recycling events could be initiated at a Venusian rift zone. We observed several instances of a tectonic regime called peel-back delamination - a form of lithospheric recycling in which the dense lithospheric mantle decouples and peels away from the weak, initially 30 km-thick crust, leaving behind a hot, thinned layer of crust at the surface (Figure 1). Delamination initiation is driven by the negative buoyancy of the lithospheric mantle and is resisted by the coupling of the plate across the Moho, the positive buoyancy of the crust arising from a range of crustal densities, and the viscous strength of the plate. Initial plate bending induces yielding and weakening in the crust, which is crucial to allow decoupling of the crust and lithospheric mantle. Unlike subduction, both positively- and negatively-buoyant plates may undergo delamination if there is sufficient negative buoyancy in the lithospheric mantle. Following a delamination event, the emplacement of hot, buoyant asthenosphere beneath the crust may have consequences for regional-scale volcanism and local tectonic deformation on Venus within the context of the regional equilibrium resurfacing hypothesis.



Typical evolution of a peel-back delamination event shown in the (i) full-scale viscosity field, (ii) local viscosity field, and (iii) local density field of reference model. (A) A 250 km-wide gap separates a 250 km-thick plate edge on the left from a 100 km-thick plate edge to the right. (B) The edge of the thicker plate bends downward due to the negative buoyancy of the lithospheric mantle. A layer of eclogite is formed in the thin layer of crust still attached to the down-going plate. (C) The lithospheric mantle continues to peel-back from the surface and thicker layers of crust are recycled due to eclogitization of the growing crustal root over the delamination hinge. The slab tip encounters phase transitions near 710 km depth and (D) is deflected upward. (E)

#### The plate necks and thins at the delamination hinge prior to slab break-off at the surface.

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# Thermochemical modeling of the lunar mantle - Effects of an initially layered composition

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The Moon was initially covered by a global magma ocean as a consequence of the Moon-forming impact. Upon cooling, the magma ocean underwent fractional solidification, which led to an initially layered composition in the lunar mantle. The aim of our work is to investigate the effects of the layered initial mantle composition on the convection and the subsequent melting of the lunar mantle.

In our work we use the mantle convection code GAIA [1] to model the thermochemical evolution of the Moon. We consider a compositionally heterogeneous mantle and compare our results with a homogeneous lunar mantle scenario. For both scenarios (i.e., homogeneous and heterogeneous mantle), we use a petrological model [2] to calculate the initial density, solidus and liquidus curves, density change due to depletion, and, in case of a heterogeneous lunar mantle, the initial temperature profile and the initial layered structure. Our models use a 2D quarter cylinder geometry. We employ an Arrhenius law to calculate the temperature and depth dependent viscosity, and we account for core cooling, radioactive decay, and mechanical mixing. The mantle composition is tracked via a particle-in-cell method [3], where tracer particles carry information about material properties such as density, melting temperature, degree of depletion, and amount of heat producing elements. We account for latent heat consumption during melting and consider both the increase of solidus and the changes in density of the residual material due to mantle depletion. Our models track the timing of the melting events and how much of the components melted.

We calculate the amount of secondary crust produced during the evolution and require that successful models fit the present-day secondary crust thickness with values between 2 and 10 km. This range accounts for basaltic lava flows that comprise less than 1% of today's crust [4] and the Mg-suite rocks, that account for about 6% to 30 %, though recent findings show that at least some rocks of the Mg-suite originated from impact melts [5].

Our results show that a model with a homogeneous initial mantle composition either produces too much crust to match today's estimates, or needs a very cold initial temperature profile, which is unlikely to be established from a solidifying magma ocean, and then produces melt too late to match the ages of the Mg-suite rocks. The heterogeneous models can match the estimates when at least part of the IBC layer takes part in the mantle convection.



Figure 1: Convection in an initially layered lunar mantle. In panel a) the initial layered composition is shown (using the density field) directly after the solidification of the lunar magma ocean, whereas in panel b) the same case is shown 500 million years later. The models use an anorthositic crust with a low thermal conductivity of 2 W  $m^{-1}K^{-1}$  and four mantle compositional layers (top to bottom): IBC = ilmenite bearing cumulates; Cpx = clinopyroxene rich cumulates; Opx = orthopyroxene rich cumulates, Olv = Olivine rich cumulates. The figure is shown to illustrate the convection in a multilayered lunar mantle in a case where IBC takes part in the convection.

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# Impact-induced crustal dichotomy on Mars

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The Martian dichotomy is one of the oldest and most distinctive geological features on the surface of Mars. It is represented by a stark difference between the northern lowlands and southern highlands, of roughly 5.5 km in topography and plausibly 25 km in crustal thickness. Despite being discovered 30 years ago, there has not been strong consensus on how the dichotomy was formed. Some of the more popular hypotheses involve a giant impact between proto-Mars and a smaller impactor, by either stripping away primordial crusts and forming a giant impact basin, or forming a large impact dome from the crystallization of impact melt into the thicker crust.

Several classes of models have been employed to investigate the formation mechanism, but are subjected to their respective model limitations. Particle-based and grid-based collision models allow studying a wide range of impact scenarios, but cannot accurately predict, from merely the impact melt distribution, the crustal formation and evolution in the subsequent millions to billions of years; on the other hand, mantle convection models can investigate the long-term evolution of the planet, but usually only consider very simplified impact scenarios. Golabek (2017) [1] demonstrates the feasibility of coupling collision models and mantle convection models, unfortunately the long-term model is only performed until 0.5 Myr.

To understand the complete geological process, we employ the results from SPH simulations [2] as the initial condition of mantle convection models, and model the 4.5 billion years of postimpact evolution of the Martian interior using the thermochemical code StagYY in 3D yin-yang geometry. This allows the tracking of impact materials distribution, the interaction between the impact-induced magma pond and surrounding mantle, and the formation of crust. We found that the mantle dynamics in these models are in broad agreement with that observed in our previous simplified 2D study [3], favouring a southern giant impact instead of the northern 'Borealis impact'. Here, we present a comparison between 2 impact scenarios with impactor radii 500 km and 750 km. In particular, we show that while a dichotomy-like crust can be reproduced in both scenarios, the different impactor sizes can lead to different mantle flow patterns hundreds of million years later, resulting in dissimilar trends of magmatism in the more recent Martian geological history.

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# Planetary surface tectonics and mantle convective regimes with grain size evolution

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To simulate Earth-like tectonic regimes, geodynamic models need an 'ad hoc' yield stress lower than any strength measurement of natural samples in brittle or plastic failure experiments. It has been suggested that grain size reduction due to dynamic recrystallization may decrease the effective strength of the lithosphere and therefore aid the onset and persistence of the mobile-lid regime. On the other hand, grain growth may have an opposite effect, impeding subduction in turn. Despite these critical aspects, the role of grain-size evolution (GSE) in global convection models with different tectonic regimes is not fully understood.

In this work, we carry out an investigation of 2D whole-mantle annulus models with composite rheology and fully-coupled GSE (Figure 1). We compare cases with varying GSE parameters to cases with constant, non-evolving grain size, and vary the yield stress to study the effect of GSE on the tectonic regime. Our models show that mantle viscosity profiles under GSE are inherently different to profiles assuming constant grain size. In this context, the lower mantle shows greater variations in viscosity than the upper mantle, with viscosity contrasts between upper and lower mantle and plume widths comparable to those of Earth in models with enhanced grain growth.

More importantly, our models show that, while enhancing grain size reduction close to the surface reduces episodicity and generally increases mobility, enhancing grain growth favors subduction generation convection as well (although episodic in many cases). This is at odds with previous conceptions of grain-size evolution-induced mobile-lid regime, where grain growth should promote healing of the lithosphere and therefore inhibit subduction. Overall, our results suggest that low temperatures at the surface (enhanced grain reduction) may result in a mobile-lid regime for Earth, while the hot surface temperatures of Venus (due to decreased grain reduction, but not increased grain growth) favor a more episodic recycling.



Figure 1. Snapshots of the (a) potential temperature, (b) viscosity and (c) grain size fields. All values are non-dimensional

### Thermal evolution of Mercury's interior

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Mercury experiences significant surface temperature variations between its polar region and its equatorial region due to its very low obliquity, a pattern that is thought to play a central role for the planet's interior evolution and thermal state. In addition, lateral variations of the crustal thickness based on the MESSENGER gravity and topography data [1] can also affect the temperature distribution of the lithosphere and mantle as it was suggested for Mars [2]. In this study, we investigate the effects of surface temperature and crustal thickness variations on the thermal evolution of the interior of Mercury. We computed the surface and CMB heat flux patterns, as well as that of the elastic lithosphere thickness and compared our results to local elastic thickness estimates (e.g., [3]).

We combine the geodynamical code GAIA [4] with the surface temperature variations and crustal thickness data similar to [2]. All simulations are done in a full 3D spherical geometry, use the extended Boussinesq Approximation, and consider core cooling and radioactive decay. The pressure- and temperature-dependent viscosity follows an Arrhenius law for diffusion creep.

We use a pressure- and temperature-dependent thermal expansivity and conductivity in the mantle [5], as well as a crust, which is enriched in heat producing elements (HPEs). We test several crustal thickness models of [1], namely model U0, V0, V3 and V4 (Fig. 1a). Additionally, our models include surface temperature variations (Fig. 1b)

We model the entire evolution of Mercury to determine the variations of core-mantle boundary and surface heat flux, as well as the mechanical lithosphere thickness, which represents an upper bound for the elastic thickness.

Our models indicate that the surface temperature variations of Mercury introduce a long-wavelength pattern on the heat flux and mechanical thickness. The crustal thickness variations and enrichment of the crust in HPE, on the other hand, lead to smaller scale perturbations that may affect the local heat flux and mechanical thickness values. We calculate local values of the mechanical lithosphere thickness during the early evolution of Mercury (Fig 1. c) in order to compare them with literature estimates of the elastic thickness (Fig 1. d) to determine which models are compatible with observations.



Fig 1: Mercury thermal evolution model. a) crustal thickness for the model V3 (Beuthe et al. 2020) ; b) surface temperature ; c) calculated mechanical thickness at 0.5 Gyr and literature data (colored triangles); d) computed mechanical thickness from thermal evolution model V3 and comparison with literature data (red zones, Caloris basin at 3.9-3.7 Ga and Discovery Rupes at 4.0 Ga).

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# Effects of the spherical annulus geometry on the thermal evolution of terrestrial planets

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Two-dimensional geometries are still widely used for thermochemical convection modeling despite the ever-increasing computing power. Although various 3-D grids are available such as the Yin-Yang grid [1] and the spiral grid [2] among others; simulations with these geometries remain highly expensive in terms of computational power and thus 2-D geometries are still preferred in most of the exploratory studies involving broader ranges of parameters. However, these 2-D geometries still present drawbacks for the thermal convection and more notably for accurate thermal evolution models of terrestrial planets, where scaling and approximations are to be made. In this scope, another 2-D geometry called "spherical annulus" has been proposed by Hernlund and Tackley, 2008 [3], which overcomes the major drawbacks of the 2-D cylindrical geometry.

In this study we implemented the 2-D spherical annulus geometry in the mantle convection code Gaia [4]. We benchmarked our implementation using steady-state simulations and compared our simulations with results from the ASPECT convection code [5]. We have performed a systematic comparison between the 2-D geometries and the spherical shell 3-D geometry for various interior structures, Rayleigh numbers and heating modes (Fig 1). Furthermore, we used the various geometries to model the thermal evolution of Mercury-like, the Moon-like, and Mars-like planets, which differ in particular in their interior structure.

The thermal evolution simulations themselves use the extended Boussinesq approximation (EBA), an Arrhenius law for the viscosity, a variable thermal conductivity between the crust and the mantle, and consider the decay of radioactive heat sources and the cooling of the core.

Our results show that the spherical annulus can better reproduce the 3-D geometry results than the 2-D cylinder geometry. For both steady-state and thermal evolution scenarios, discrepancies between the cylindrical geometry and the spherical shell geometry are largest for aspect ratios (inner radius / outer radius) smaller than 0.4.

We performed an extensive comparison between the 2-D and the 3-D geometries for both steadystate and thermal evolution calculations to illustrate the differences between the spherical annulus, cylindrical, and spherical shell geometry.



Fig 1: Comparison between 2-D spherical annulus (top row), respectively 2-D cylindrical (bottom row), and 3-D spherical shell geometry. The panels show the relative error to 3-D results for the mean temperature (left column), RMS velocity (middle column), and top Nusselt number (right column). The tests cover a range of radius ratios (from 0.2 to 0.8) and Rayleigh numbers (from 104 to 107). All cases shown here are heated from below and also consider internal heat sources.

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# Magma oceanography of the dense, ultrashort-period sub-Earth GJ 367b

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The dawn of high-resolution observations with the James Webb Space Telescope will enable spatially resolved observations of ultrashort-period rocky exoplanets. Some of these planets orbit so closely to their star that they lack an atmosphere [1], which gives direct access to their surfaces and opens a window to infer their geodynamics [2]. The physical parameters of the ultrashortperiod sub-Earth GJ 367b have been observationally constrained to a planetary radius of about 0.72 to 0.75 Earth-radii and a mass between 0.48 and 0.55 Earth-masses, implying a density of 6200 to 8500 kg/m 3 [3, 4], which puts this planet in a Mercury-like interior regime with a thin mantle overlying a fractionally large core. The dayside temperature ranges between 1500 to 1800 K, thus suggesting the presence of a permanent magma ocean or dayside magma pond on the surface, induced by stellar irradiation. The large uncertainty on the age of the stellar system, between 30 Myr [4] and about 8 Gyr [3], however, introduce severe uncertainties related to the compositional and thermal evolution of the planetary mantle. In this study we perform global 2D spherical annulus StagYY simulations [5, 6] of solid state mantle convection and surface melting with the goal to constrain the geometric and compositional properties of the planet. Constraining the spatial dimensions of thermodynamic properties of partially molten, atmosphere-less planets like GJ 367b offers unique opportunities to constrain the compositional fractionation during magma ocean epochs and provides avenues to constrain the delivery and loss cycle of atmophile elements on strongly irradiated exoplanets.

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# Evolution of the convective regimes at high Rayleigh number in a laboratory planetary mantle.

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Ludox colloidal dispersions have a complex rheology with viscous, elastic, plastic and brittle properties that depend on their water content [1]. Such a variety of behaviours makes these dispersions a relevant model system to study the different convective regimes in a complex fluid, and enables to reproduce the phenomenon of subduction in the laboratory. Rayleigh numbers involved have a similar order of magnitude in the laboratory experiments and in the mantle. Prandtl numbers are much greater than one, insuring neglectable inertial effects. Ludox is thus a promising analog system to study convection in planetary mantles [2, 3], as the mantle can be described as a complex fluid whose rheology depends on temperature.

Following the convection can be achieved using standard fluids mechanics methods, like PIV and shadowgraphy. A complementary approach is to use a thermal IR camera to measure the emissivity of the surface, which is linked to its temperature but also depends on other variables such as the topography of the surface or its composition.

In a first time, to test our experimental setup, we studied the simpler case of evaporation of a water tank heated from below: the surface remains flat, and the composition is constant ; the emissivity thus only depends on the temperature of the surface. We observed the evolution of the geometry of convection along time (from plumes to cells) and a transition between a Rayleigh-Benard dominated regime and a Benard-Marangoni dominated regime due to the presence of thermocapillary effects (that are not desired to model the mantle).

In a second time, we use the same protocol with Ludox. This time, in addition to the hot rising plumes, we observe the water content decreases and a stagnant lid forms at the surface. This lid folds before subducting. In this case, the temperature displayed by the camera is an effective temperature, resulting from the coupling of the effects of temperature, composition and topography. However, these three effects have different statistical signatures.



Figure 1: Left: Thermal plumes rising to the surface of a Ludox tank heated from below at 30°C. Right: Deformed surface of the same Ludox suspension after 10 hours of drying, just before a subduction event.

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# Modelling coupled fluid mechanics and thermo-chemistry of magma ocean crystallisation: application to the lunar magma ocean

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During planetary formation, massive amounts of accretional energy can lead to the formation of a global magma ocean. Understanding the dynamics of magma ocean crystallisation during planetary cooling can help constrain the initial mantle structure of early planetary bodies. However, most studies either focus on the fluid dynamics of a cooling magma ocean (e.g., Maurice et al. 2017) or on the thermo-chemistry of magma ocean crystallisation (e.g., Johnson et al. 2021). Accounting for reaction-transport dynamics emerging from coupled mechanics and chemistry in numerical models is essential to resolve convection and crystal-melt segregation rates, and thus the resulting interior structure. However, coupled models are challenging to achieve, especially with multi-component chemistry and due to the limited experimental data on the crystallisation of magma oceans.

We develop a two-phase, 6-component model in a 2D rectangular domain based on Keller & Suckale (2019). Magma ocean convection is modelled using Stokes equations while crystal settling is calculated using a form of hindered Stokes law. The fluid mechanics model is coupled with a thermo-chemical model of evolving temperature, phase proportions, and phase compositions to form a reactive transport model, following Keller & Katz (2016). We apply this model to the lunar magma ocean (LMO) by describing the melt and crystal compositions with 6 pseudo-components (approximating forsterite-fayalite, orthopyroxene-clinopyroxene and anorthite-albite mineral systems). We develop a Markov-Chain Monte Carlo method to calibrate melting temperature and composition of each component to fractional crystallisation experiments for a Taylor Whole Moon composition (Schmidt & Krättli 2022).

Preliminary tests show that the 6-component melting model calibrated to experimental data can be successfully implemented in the reactive transport model. This model then allows for the investigation of timescales of solidification and potential density and compositional stratification due to fractional crystallisation upon mantle solidification. The small size of the Moon and its relatively well constrained magma ocean history, make the LMO an excellent case study to apply the model. However, with the aid of new experimental data for larger and chemically different planets, such as Mars, this model can provide more general insight into the early evolution of terrestrial bodies.

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# Convection in Europa's icy shell: numerical simulations with composite rheology and dynamic grain size evolution

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Europa's hydrosphere probably features an icy crust of some to some tens of kilometer thickness that overlies a liquid ocean. Europa's surface appears heavily deformed and the low crater density suggests a low mean surface age of 60-100 Myr [1], implying active resurfacing. Previous works have even proposed a plate-tectonic-like nature of Europa's tectonics, including subduction-like processes [2]. While this requires confirmation by future missions, convection in Europa's icy shell is a viable mechanism to drive such processes and would also impact surface-ocean exchange and thus Europa's habitability potential. However, the style of convection and its link to resurfacing is poorly understood. Therefore, we use 2D numerical simulations using the code StagYY [3] to shed light on these aspects. We implement a composite rheology featuring the different slip mechanisms identified for ice [4] and including grain-size evolution (GSE). We test basally heated and also tidally heated scenarios in a 20 km-thick shell and vary the parameters governing the deformation mechanism (diffusion creep, basal slip, grain-boundary sliding, dislocation creep) and GSE (grain growth vs. reduction).

Without imposing a yield stress, we preliminary find that grain size reduces to <40  $\mu$ m in the top several km, while in the deeper warmer layers grain size is on the order of centimeters. However, the small grain size at shallow depth seems secondary for the viscosity, as the temperature dependence of viscosity is dominant. Varying the magnitudes of grain growth and reduction changes the grain size in the deeper shell, which is reflected in the interior viscosity and can in some cases shutdown convection. The dominant deformation mechanism in the ice shell strongly depends on the reference stresses (equivalent to different pre-factors in the Arrhenius law) for the different deformation mechanisms. Allowing for substantial dislocation creep can reduce boundary layer thickness by several km. Adding tidal heating further reduces this thickness, but also increases internal temperature to the solidus for tidal heating rates  $\geq 10^{-5}$ W/m 3 , if tidal heating is assumed optimal at the interior viscosity (here  $10^{13}$  Pa s). All cases without yield stress display no surface deformation or mobility, consequently a very old surface. This conflicts with Europa's young surface, unless other processes (e.g., cryovolcanism) are responsible for the resurfacing. In the next step, we therefore compute cases allowing for plastic deformation at shallow depths to induce convection-driven surface mobility.

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## **Dislocation creep triggered by giant impacts**

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Temperature-dependent visco-plastic rheologies are commonly used to perform numerical simulations of planetary mantle convection on various planets. This generally seems like a reasonable thing to do as there are only evidences of non-Newtonian rheologies being active in the Earth's upper mantle where huge slabs generate large stresses believed to be necessary to activate dislocation motion. Plate tectonics being absent on all other rocky bodies of the solar system, one can expect that ambient mantle convective stresses must be quite lower than those of the Earth. Yet, there is the exception of very dramatic events which have been shown to have happened at the very formation of our planetary system. When giant impacts occurred, even on small planets, surely stresses large enough to activate dislocation creep must have been reached.

In this study, we investigate the effect of composite rheologies on the thermo-compositional equilibration of post giant impact anomalies using the convection code StagYY. We expect the spread of impact-related temperature anomalies to reach much further when a non-Newtonian rheology is employed. This has important implications on the morphology of early crust production.

We use the convection code StagYY solving for mantle compressible convection with self-consistent melting and basaltic crust production and a free surface. A special treatment for magma ocean cooling is employed based on a drastically increase magma effective thermal conductivity. This allows for a realistic cooling time scale necessary to not over-estimate the lateral spread of the original heat anomaly generated by the parameterised impact. When a low enough degree of melting is reached, basaltic melts are transported to the surface of the domain, forming the primordial crustal material possibly still observable today on various rocky bodies of the solar system.

## Factors influencing radiogenic heat source and volatile redistribution in rocky planets

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The thermal evolution and atmosphere development of terrestrial planets depends on a number of processes in the mantle and lithosphere. Radiogenic elements like Uranium, Thorium, or Potassium, for instance, contribute large amounts of heating to a planet's mantle. However, these heat producing elements (HPE) are incompatible in solid mantle rocks and are redistributed into melt upon partial melting events. Partition coefficients indicate how many of these incompatible elements are redistributed. However, they need to be applied carefully, since they can change by multiple orders of magnitude along the peridotite solidus from 0-15 GPa (Fig. 1, Schmidt and Noack, 2021). Due to a lack of high-pressure experimental data and models, partition coefficients were generally taken as constant values. If the HPE-enriched melt is less dense than the surrounding material, it rises towards the surface and causes a shift in the heat budget between a planet's crust and mantle. In turn, this shift influences the melt production and the growth rate of the lithosphere and crust. The outgassing of H<sub>2</sub>O follows the same mechanism, but unlike HPEs, it is outgassed and contributes to the atmospheric layer on top of the crust.

In this study, we developed a 1D interior evolution code for terrestrial planets which models, amongst others, the thermal evolution of a planet, thickness of crust and lithosphere, outgassing of  $H_2O$  and  $CO_2$ , and the overall concentration of the redistributed HPEs for several planets and moons inside our solar system. Based on the partition coefficient parameterization of Schmidt and Noack (2021), we included P-T-X dependent partition coefficient calculations in our 1D model and compare the results with our model using constant partition coefficients from the literature. Additionally, we vary other starting parameters and again compare how this affects the amount of the elements that were redistributed into the crust or outgassed into the atmosphere. By constraining the effects of depth- dependent redistribution and variable starting parameters, the study can help us understanding for which types of terrestrial planets the more complex approach is relevant.



Fig. 1: Thermodynamic model for sodium partitioning in clinopyroxene/melt. Along the peridotite solidus, the partition coefficients vary up to two orders of magnitude (Schmidt and Noack, 2021).

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# Exploring the effects of terrestrial exoplanet bulk composition on long-term planetary evolution

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The catalog of known exoplanets has increased vastly since the first detection in 1995, exoplanets show a wide range in properties such as size and composition. The composition of a terrestrial planet modulates many properties, including core size, mantle rheology, and mantle melting behavior. However, the full effect of compositional influence on terrestrial planet evolution has only recently reached a level of maturity that it can now be applied to exoplanets. We attempt to constrain the possible range of bulk terrestrial exoplanet compositions, and explore the effects of bulk composition within this range using a geodynamical model.

We constrain the range of bulk terrestrial exoplanets based on stellar compositions in the solar neighborhood (Hinkel+, 2014) by considering planets as devolatized stars (i.e., stars that have lost their volatile elements, such as H and He; Wang+ 2019). We identify 20 end-member bulk planet compositions that span the full range of compositional diversity. Bulk composition is given in terms of the most common elements in rocky planets: Fe, Mg, Si, O, Ca, Al, Na, Ni, and S. Relative core size is determined by considering iron, nickel, and sulphur abundances, assuming constant bulk planet oxygen fugacity. Core composition is subtracted from the bulk to determine mantle composition.

We explore the effects of bulk planet composition on long-term interior evolution using a geodynamical model, StagYY (Tackley, 2008), for planets composed of our 20 end-member compositions. We account for the various mantle compositions by including lookup tables for physical mantle properties calculated by Perple\_X (Connoly, 2005) with the thermodynamic database by Stixrude and Lithgow-Bertelloni (2022). We adjust the melting calculation scheme to account for varying basalt fraction and iron abundances in the mantle. Further, we explore the propensity of each planet towards plate tectonics-like behavior, stagnant lid-like behavior, or behavior that falls under a different dynamic regime.

Generally, Earth has an average composition for most elements, except it is relatively rich in iron, and therefore it has an above average core size. Our preliminary results show that core size affects convective vigor, and thus thermal evolution of the interior. We further find major differences for planets with different Mg/Si-ratios, where planets with lower Mg/Si than Earth are richer in bridgmanite and will have a significantly stronger mantle, impeding cooling on planetary lifetimes. Meanwhile, high-Mg/Si planets have weaker upper mantles, containing wustite, impacting surface mobility. Therefore, bulk planet composition has a significant effect on planetary evolution.

## Initiation, Interaction, and Suppression of Mantle Plumes on Venus-analog Planet

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Although Venus has roughly the same composition, size, and distance from the Sun as the Earth, it has a unique topographic landscape of both Large Igneous Provinces (L.I.P.s) which are present on Earth, and coronea, fractured and circular regions of smaller volcanic upwellings, which are not (Smrekar and Stofan, 1999). Additionally, the tectonic history and mobility of Venus' surface is not understood but differs greatly from Earth with discrete tectonic plates forming at mid-ocean ridges and being recycled at subduction zones. Research since the Magellan mission in the 1990s suggests Venus may have processes analogous to Earth-type subduction of its lithosphere (Schubert and Sandwell, 1995). The recycling of cold lithosphere to Venus' core-mantle boundary may hold the key to explaining the diversity of upwellings that lead to a dichotomy of regionally-close L.I.P.s and coronae formations (Davaille et al., 2017; Robin et al., 2007).

Numerical models solving for the conservation of mass, momentum, and energy of a Buossinesq fluid are run using the planetary-convection code StagYY (Tackley, 2008) on the NSF Expanse supercomputer. The domain of the model is a two-dimensional hemi-spherical annulus of a terrestrial planetary mantle. We initialize the mantle at potential temperatures of 1600 K, 1700 K, and 1800 K, and the model is heated from the bottom 100, 200, 300, and 400 K above the background mantle temperature. This sharp temperature gradient produces a thermal boundary layer of fluid at the core-mantle boundary, from which mantle plumes form and ascend. Although our expectation was that such modest temperature differences would only allow the formation of small diapirs (thermal blobs with no trailing conduit), we observe the strongly temperature-dependent viscosity allows for small plumes (with heads and conduits) to form.

We explore how the presence of a segment of cold, viscous lithosphere initiated near the coremantle boundary modulates mantle plume initiation. In combination with depth-dependent viscosity increasing with depth, we observe and characterize various regimes of plume formation, interaction, and suppression. We consider what scenarios may lead to the development of a volcanic dichotomy on the planet's surface (Robin et al, 2007).

## Geoid and Topography on Venus: Static or Dynamic?

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On Earth, the long-wavelength geoid and total surface topography are poorly correlated, with the interpretation that total surface topography is due mainly to the ocean-continent dichotomy whereas the geoid reflects density anomalies deep in the mantle caused primarily by subducted slabs. On Venus, in contrast, the geoid and topography are well correlated, indicating a more direct connection between convection and the lithosphere and crust. It is unclear what causes the geoid and topography variations on Venus. Two end-member origins of geoid and topography variations have been proposed:

(1) Deep-seated (i.e. below the lithosphere) density anomalies associated with mantle convection, which may require a recent global lithospheric overturn to be significant (e.g. Armann and Tackley, 2012 JGR; King, 2018 JGR; Rolf et al., 2018 Icarus).

(2) Variations in lithosphere and crustal thickness that are isostatically compensated - the so-called "isostatic stagnant lid approximation" (Orth and Solomatov, 2011 G3, 2012 G3), which was demonstrated to be consistent with simple isochemical stagnant-lid convection experiments.

In this study, we analyse dynamical two-dimensional thermo-chemical models of Venus' mantle and crust that include melting and crustal production, multiple composition-dependent phase transitions and strongly variable viscosity, to test whether variations in crust and lithosphere thickness explain most of the geoid and topography, or whether they are caused mostly by density variations below the lithosphere.

Results show that generally, most of the geoid and topography signal originates from the top 300 km of the domain. Exceptions are the very longest geoid wavelengths, where some deep mantle influence is found, and for the period immediately following a lithospheric overturn, during which substantial mass anomalies exist in the deep mantle.

Thus, in the stagnant lid regime or after long periods of quiescence in an episodic overturn regime, it is concluded that, except at the very longest wavelengths, the isostatic stagnant lid approximation is correct, i.e. most of the geoid and topography signal originates in the lithosphere. This is easy to understand because during stagnant lid convection, mass anomalies in the deep mantle are much smaller than they are when subduction or global lithospheric overturn is taking place. A shallow origin for geoid and topography implies that they are not sensitive to mantle viscosity profile.

Further details may be found in the Masters Thesis of Rens. S. Elbertsen (U. Utrecht, 2021).

## New tectonic and resurfacing mechanisms for Venus

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To explain Venus' young surface age and lack of plate tectonics, Venus' tectonic regime has often been proposed to be either an episodic-lid regime with global lithospheric overturns, or an equilibrium resurfacing regime with numerous volcanic and tectonic activities. However, stratigraphic analysis suggests that Venus' surface tectonics could be a combination of these two endmember models, with a global resurfacing event that created most of the crust, followed by tectonic and volcanic activities until now. Recent analyses of Venus' satellite images also suggest widespread lithospheric mobility in the lowland basins. These observations cannot be explained by the episodic-lid tectonic regime obtained in previous geodynamic models (e.g. Armann & Tackley, JGR 2012) as these exhibit negligible crustal deformation between resurfacing events. Here we model Venus' thermochemical evolution using the geodynamic code StagYY in a 2D spherical annulus geometry. Compared to previous global models, the new parameters are:

- 1. **More realistic rheology**: previous models assumed olivine diffusion creep for the entire crust and mantle: (i) An experiment-based crustal rheology, based on An75 plagioclase (both diffusion and dislocation creep) and used in regional geodynamic models that successfully reproduce corona/nova features (Gülcher et al., Nature Geoscience 2020), is applied in this study. (ii) Dislocation creep is included throughout the entire mantle.
- 2. Intrusive magmatism. For magmatism, previous Venus models assume either no melting at all, or pure eruptive magmatism. It was previously shown that high intrusion fractions lead to a new tectonic regime: the plutonic-squishy-lid regime (Lourenco et al., Nature Geoscience 2018; GCubed 2020).

We find that tectonics is strongly affected by crustal rheology. With a "weak" plagioclase crust, the surface mobility is continuous rather than episodic-lid as in olivine-crust models. Magmatic resurfacings are short-lived and randomly-located, leading to a rather uniform resurfacing rate. Internally, the composition-dependent density profile results in a "basalt barrier" at the mantle transition zone (Papuc & Davies, Icarus 2012), which strongly affects Venus' mantle evolution. Only strong plumes can penetrate this basalt barrier and cause global overturns.

We also find two new mechanisms for global overturns:

- 1. Lithospheric overturns without plasticity: A combination of plagioclase crustal rheology and dislocation creep can weaken the lithosphere sufficiently. This is important because for olivine diffusion-creep rheology, plastic failure parameters need to be set unrealistically low.
- 2. Global resurfacing without lithospheric overturn: In stagnant-lid models, the basalt barrier mechanism can cause global internal episodic overturns that generate massive melting and global crustal production.



Figure 1: The evolution of average surface age, average crustal thickness (a, b), and surface mobility (c, d) for two models without plastic yielding.

# Is the volatile release contributing to early Earth's atmosphere underestimated?

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The intrusive proportion of the total magma production on Earth is about 80%. Hence, it can be assumed that the release of volatiles from intrusions significantly contributes to the total outgassing into the atmosphere. Nevertheless, intrusive volatile release is commonly neglected in studies modelling the composition of the early atmosphere. Therefore, we suggest that the volatile release on early Earth is underestimated.

An emplaced magma body progressively crystallizes due to cooling. The precipitation of certain minerals fractionates the primitive mantle over time by incorporation of compatible elements into the crystal lattice. In contrast, incompatible elements and molecules, including volatiles like H2O and CO2 are precluded from the crystal lattice due to their unsuitable ion radius or charge. Thus, ongoing crystallization likely leads to an oversaturation of volatiles in the remaining melt and an enhanced exsolution.

In our study, we simulate the partitioning, solubility and release of H2O and CO2 from a magma body emplaced at different depths within the lithosphere. Additionally, we take the possibility of melt ascent and the formation of hydrous minerals into account. According to our simulations the release of H2O and CO2 from an intrusive magma body is possible within the whole lithosphere. However, the release strongly depends on the initial volatile budget, the formation of hydrous phases, the depth of the intrusion and the buoyancy of the melt. Considering all these factors, our model suggests that about 0 - 85% H2O and 100% CO2 can be released from mafic intrusions. This renders the incorporation of intrusive volatile release mandatory in order to determine the volatile fluxes and the composition of early Earth's atmosphere.

How does a subduction zone initiate at present-day conditions? New insights from a global compilation of Cenozoic events and from numerical studies of the simple set-up of a transform fault undergoing compression

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The process of subduction initiation, is still poorly constrained and caused a great deal of controversy such as: Can a subduction zone initiate there without any external forcing? Is the thicker plate really the more likely to subduct? To try to answer these questions, a database of 70 cases of Cenozoic subduction zone initiation has recently been built and analysed. We find that initiation of subduction zone succeeds in reaching the mature stage for 72% of the cases, usually in less than ~15 Myr, and that compositional heterogeneities are basic to localise convergence. Interestingly, we show that the plate age offset at the convergence onset is very low (close to zero) in half the cases; otherwise the infant lower plate is equally the thicker (and denser) one or the thinner one. These last observations indicate that the buoyancy contrast may not be the main parameter to determine the subduction zone polarity.

Next, we consider the case of an oceanic transform fault (TF) or fracture zone to investigate the conditions leading to subduction initiation, first because this geological set-up is the simplest to investigate, and second because transform boundaries are the most frequent configurations where subduction zones initiated during the Cenozoic. Even if subduction initiation is intrinsically a 3D process, 2-D numerical thermo-mechanical simulations were run to be able to explore numerous key parameters.

We first perform a parametric study of the feasibility of 'spontaneous' subduction initiation, i.e., lithospheric gravitational collapse, at a TF. We show that the main mechanical parameters have to be tuned to an extreme value to trigger the lithospheric instability. We compare the modelled process with records of subduction infancy, for the 3 geological candidates of 'spontaneous' subduction initiation, that are Izu–Bonin–Mariana, Yap, and Matthew and Hunter, and conclude that this process of initiation at a TF to reach subduction zone maturity is unlikely in modern Earth conditions.

At last, we simulate normal convergence symmetrically imposed on the two oceanic plates forming the TF to study the 'forced' mode of subduction initiation. We find that the success of initiation, as well as the subduction polarity (defined by the down-going plate) strongly depend on the plate age pair and on the initial structure of the TF. Surprisingly, a high plate age offset at the TF does not promote the thick plate subduction if the lithospheres are not particularly weakened. Instead, the range of conditions leading to the old plate subduction is quite limited, whereas the subduction of the young plate is much more frequently simulated. We infer that the rheological properties and the plate ability to be deformed and sheared may be the first order parameters controlling the subduction zone polarity for rather stiff lithospheres. We finally show that the model predictions are in good agreement with different Cenozoic records (Gagua, Mussau, and Hjort).

## **Volatile Recycling in the Lesser Antilles Arc**

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Volatiles exert a key influence on subduction and its associated processes and hazards, including the formation of continental crust, the concentration of ore deposits and the occurrence of volcanism and earthquakes. Most of our understanding of volatile recycling by subduction derives from the study of the circum-Pacific where lithosphere formed at fast spreading ridges subducts. However, slow-spread lithosphere is likely more substantially and variably hydrated because part of the spreading is tectonically rather than magmatically accommodated. This motivated project VoiLA to study Volatile recycling in the Lesser Antilles Arc (LAA), where slow-spread lithosphere from Atlantic and Proto-Caribbean oceanic domains is subducting.

Our wide-angle studies on the incoming plate show that it comprises about 50% tectonic and 50% magmatic crust, with the former more pervasively hydrated due to the formation of serpentinite. Additional lithospheric hydration occurs at some fracture zones and non-transform offsets, as well as during outer-rise plate bending.

Using local earthquake tomography and seismicity, we can map spatial variations in the hydration of the plate that descends below the arc. Most fluids from magmatic crust are released around 80 km depth, while serpentinite carries fluids down to depths of up to 150 km. Once released from the slab, these fluids get transported further downward in a thick cold thermal boundary layer overlying the relatively slowly subducting old and cold plate, before being released below the back-arc. Attenuation and surface-wave tomography reveal back-arc mantle anomalies that we attribute to fluid-assisted melting that is particularly enhanced behind the central arc due to the strongly tectonised domain boundary between Atlantic and Proto-Caribbean lithosphere that subducts there.

The wedge melts rise and pond below the back-arc upper plate giving rise to a prominent LAB imaged in receiver functions. The melts then migrate from the back-arc towards the arc, probably aided by gradients in upper plate thickness and the corner flow driven by the subducting plate. This pathway of fluids and melts can explain enhanced serpentinite-fluid fingerprints in boron isotopes of magmas from the north-central islands. To reach the arc, we propose that magmas exploit structures formed in a previous phase of back-arc spreading before the arc jumped into its own backarc, in response to a significant decrease in subducting plate age as a large-offset transform arrived at the trench.

Thus, our combined seismic imaging, geochemical analyses and gravity and magnetic mapping and modelling of plate motions reveals how fluids are moved into and out of the LAA subduction zone along more complex pathways than usually considered. Some parts of the process are particularly clearly seen in the LAA because of the highly variable hydration of the incoming plate and its slow convergence. This illustrates how the position of the arc is the result of both plate-driven mantle flow and upper plate structure conditioned by its previous tectonic evolution, while the variable hydration of the incoming plate and subsequent flow pathways govern how volcanic productivity varies along arc and through time.



Schematic overview of the VoiLA project

## A two-phase flow perspective on melt transport beneath midoceanic ridges

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At mid-ocean ridges, oceanic crust is emplaced in a narrow neovolcanic region on the seafloor, whereas basaltic melt that forms this oceanic crust is generated in a wide region beneath as suggested by a few geophysical surveys. The combined observations suggest that melt generated in a wide region at depths has to be transported horizontally to a small region at the surface. We present results from a suite of two-phase models applied to the mid-ocean ridges, varying half-spreading rate and intrinsic mantle permeability using new openly available models, with the goal of understanding melt focusing beneath mid-ocean ridges and its relevance to the lithosphere-asthenosphere boundary (LAB). Three distinct melt focusing mechanisms are recognized in these models: 1) melting pressure focusing, 2) decompaction layers and 3) ridge suction, of which the first two play dominant roles in focusing melt. All three of these mechanisms exist in the fundamental two phase flow formulation but the manifestation depends largely on the choice of rheological model.

Recent debate has focused on whether sea level changes — driven by Milankovitch glacial cycles — generate the abyssal hill fabric of the ocean floor by modulating mid-ocean ridge magma supply. We use 40 m-resolution bathymetric data collected over hundreds of square kilometers during the search for Malaysia Airlines Flight 370 on the flank of the Southeast Indian Ridge, which provides a record of crustal accretion from 11–23 Ma. Spectra calculated from the data show a characteristic timescale of 300–400 kyr and no evidence for periodicity coinciding with glacial cycles. This characteristic timescale could be explained by fluctuations in melt supply and the amount of faulting, leading to variations in crustal thickness. We show that this timescale of variation is consistent with porosity waves observed in a two-phase flow model, which persist over millions of years. Further exploration of the two-phase flow models show that persistent melt-rich porosity waves are responsible for the ocean floor fabric at periods of 100 kyrs and longer, except in the case of fast-spreading ridges. For periods longer than 100 kyrs, spectral energy is notably present at large mantle permeabilities regardless of spreading rates.



Figure 1: Modified mobility number,  $Mo = \frac{w_0}{U_0} \frac{U_c}{U_0}$  for varying intrinsic permeability,  $K_0$ , and half spreading rate,  $U_0$ . Black dots are the models that have persistent porosity waves. White dots are the models that are lacking in persistent porosity waves. Dots circled yellow are from Parnell, Sim and Olive, 2020 and circled red from Sim et al 2020. The contour of 45 indicates the critical  $w_0/U_0$  where the models transition from having persistent porosity waves to none. Adapted from Sim 2022.

## Subduction initiation at passive margins: Insights from 3D numerical modeling

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Some of previous studies (e.g., 1,2) noted the difficulty of conversion of passive margins into active ones due to the large force, which is needed to break and bend the old lithosphere. They suggested that the favourable locations for subduction initiation are pre-existing weakness zones in the lithosphere such as mid-oceanic transform faults/fracture zones. However, modelling studies have proposed some weakening mechanisms such as water weakening (3), weakening due to grain damage (4) and mantle suction flow (5), facilitating subduction initiation at passive margins. Mantle suction induced subduction initiation was investigated in our previous work (5) using 2D numerical models. In this study, we aim to expand our previous study by using 3D numerical experiments. We investigate the possibility of destabilising of a passive margin by mantle suction force. We also evaluate the possible role of STEP (Subduction-Transform-Edge-Propagator) faults on conversion of passive margins into subduction zones. To this purpose, we setup two series of 3D models. In the first set of experiments, we examine whether suction force alone is able to break the lithosphere and initiate a new subduction zone. Our model domain is a cuboid of 2000\*1000\*400 km3, consisting of an old oceanic lithosphere, a continental plate and asthenosphere till depth of 400 km (Figure a). In the second set of models we include a STEP fault to the midel of model to investigate its effect on subduction initiation (Figure b). The STEP fault is defined by a weak low-viscosity zone in the middle of model.

Our preliminary results indicate that from the earliest stage of deformation, continental crust thrusts over the oceanic lithosphere. At the same time, mantle suction force imposes some shear stresses below the lithosphere. Over a period of few tens of million years, the stresses exceed the yield stress, resulting in breaking of the oceanic plate. It follows by sinking of the oceanic plate into the mantle and eventually subduction initiation at passive margin. In our experiments subduction initiates at more than 30 Myr, indicating difficulty in conversion of passive margins into active ones. We believe that at some Atlantic passive margins such as those in the North of South Sandwich subduction zone, Southwest of Iberia and North of Caribbean region, where active neighboring subduction zones and/or detached slabs within the mantle induce considerable suction forces, subdction will initiate in few tens of million years.

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Figure: Model setup. (a) Initial model setup of the first set of experiments. (b) Initial model setup of the second set of experiments. In (a) and (b) the upper panels show the compositional field (

## Continental slivers in oceanic transform faults controlled by tectonic inheritance

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The ocean floor shows variable morphological features, transtensional and transpressional structures, magmatic and amagmatic domains. Surprisingly, continental blocks separated from the continental margins from 100s or 1000s km distance have been occasionally reported, however, their origin remains controversial (e.g. Palmiotto et al. 2016).

We conducted 3D magmatic-thermo-mechanical numerical experiments with the code I3ELVIS (Gerya et al. 2013; Balazs et al. 2022) to simulate the dynamics of continental rifting, continental transform fault zone formation and persistent oceanic transform faults. Numerical modelling results allow to explain the first order observations from passive and transform margins, such as diachronous incipient rifting, strain localization into individual oblique rift basins and the opening of structurally separate oceanic basins. Our models also show the evolution of continental blocks between oceanic spreading ridges bounded by strike-slip fault zones inherited from the preceding continental rifting stage. The formation of such continental slivers is controlled by the relative timing between the onset of oceanic spreading and the strike-slip fault zones formation. This is connected to the rheology of the plates and linked to different thermal gradients, divergence velocities and surface processes. Our model results are compared with observational data from the Romanche transform of the Equatorial Atlantic, the East Greenland Ridge of the Northern Atlantic and the Zabargad Islands in the Red Sea.



Rock composition (left) and effective viscosity (right) results after 13 Myr of model run

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### **Dynamics of subduction initiation with respect to continents**

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Plate tectonics is a unique feature of Earth, which has played an important role in the physical, thermal, and chemical process of this planet. Despite its importance, geoscientists know very little about how and why plate tectonics takes place on Earth. Different lines of evidence from the geologic record suggest the link between preceding continental crust formation and subduction initiation. Moreover, the rocks from Acasta Gneiss Complex even support the idea that incipient continental blocks act as nuclei for subduction.

We used numerical models of mantle convection with an imposed continental block to test whether continents facilitate subduction initiation due to the stress developed at their margin by assuming a grain-damage rheology, so that weak shear zones form by grain size reduction driven by the deformational work done by mantle convection. Our result show that including a continent does not contribute to the remarkable enhancement in total time damage or plate speed, but stresses are modestly enhanced, and they lead to additional grain damage and rheological weakening. We developed a scaling law for the stress enhancement due to a continental block as a function of the model parameters: (1) continental thickness; (2) viscosity activation energy; (3) Rayleigh number; and (4) viscosity jump from mantle to a continent.

Subduction also does not preferentially initiate at the continental margin, contrary to another plastic model that has proposed buoyant continents spread and it leads to subduction initiation at the continent margin. The model results naturally lead to a question of where subduction initiates. We developed a novel approach of tracking subduction zone in numerical mantle convection models by identifying convergence zones in the lithosphere. Using this newly developed method, we find subduction zone locations with respect to the continental margins from the initiation to the termination. The results can be used for both early Earth and modern Earth as this study focus on the fundamental physical principles of subduction initiation.

## **Evolution of the Sunda Plate topography by subduction interactions in early Miocene**

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The Sunda Plate has shaped itself in a complex tectonic framework, driven by the interactions of multiple subduction zones in its history, which is currently bounded by two major N–S trending active trenches: Andaman-Sumatra-Java and Philippines on its western and eastern margins, respectively. The inter-trench distance (ITD,  $\lambda$ ) varies from 3000 to 500 km for North to South, across the trench perpendicular segments of Sunda plate. We consider six E-W transects to account for an along-trench variation of inter-trench distance with observed subduction rate (Vc) and shallow-depth (200–300 km) slab dip ( $\alpha$ ) in our 2-D numerical experiments. Our experiments reveal that the deviatoric stress fields and the topographic patterns are found to strongly depend on  $\lambda$ . For large ITDs ( $\lambda = 2000-3000$  km), the overriding plate develops dominantly tensile stresses in its central zone, forming low topographic elevations. Decreasing  $\lambda$  results in a transition from extensional to contractional deformation and promotes topographic uplift in the southern part. We explain these effects of  $\lambda$  in terms of the asthenospheric flow vortex patterns produced by the subducting slabs. Large  $\lambda$  (2000-3000 km) generates non-interacting flow vortices, located close to the two trenches, leaving the mantle region beneath the overriding plate weakly perturbed. In contrast, small  $\lambda$  results in their strong interaction to produce a passive mantle upwelling zone (evident from geophysical observations as well), which facilitates the overriding plate to gain a higher topographic elevation. The stress field predicted from our model is validated with the observed stress patterns. The thermomechanical computational fluid dynamic models reveal that the in-dip double-subduction dynamics has controlled the first-order 3-D topography of this plate. We also interpolate a 3-D topographic surface and vertical uplift rates from the serial model sections and compare them with the observed surface topography of the Sunda Plate.



Fig 1. (a) to (f) Isotherm patterns obtained from six across-trench sections of the Sunda plate with decreasing inter-trench distance. Note that the mantle upwelling beneath the overriding plate is evident from the isotherm bulges, where the upwelling becomes more focused and intense for lower  $\lambda$  values.

## **3D Modeling of Dynamics in the Hikurangi-Kermadec Subduc**tion System

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Subduction is a fundamental component of plate tectonics, where oceanic lithosphere is returned into the deep mantle. This process produces both abundant silicic volcanism in the overriding plate and extensive seismic activity along the plate interface, which in some cases may produce megathrust events. A wide range of observations suggest both the characteristics of volcanism and earthquake activity through time are significantly influenced by the transport and release of volatile phases (i.e, H20, CO2) from the downgoing slab. Thus constraining the volatile cycle in subduction systems is critical for understanding natural hazards and larger scale geodynamic processes. Here, we present preliminary work towards building geodynamic simulations of volatile cycling through the Hikarangui subduction system in New Zealand, which is host to both abundant silicic volcanism, inferred megathrust events, and ample evidence for large amounts of fluids within the downgoing slab, in the convective wedge, and in the overriding plate as inferred from volcanism. While the models presented do not yet specifically contain volatiles and associated transport processes, we have constructed an advanced 3D thermal-mechanical model where the resulting thermal and solid (velocity, pressure) characteristics will provide the necessary basis for examining hydration/dehydration reactions and coupled two-phase flow calculations.

We model the dynamics of the Hikurangi-Kermadec system in a 3D Cartesian box using the open source finite element code ASPECT. The initial 3D compositional and thermal structure of the downgoing plate, overriding plate, and asthenosphere are collated with the Geodynamic World Builder software package. Accurate slab geometry, with along-strike and down dip variations, is achieved using depth to slab top data taken from the Slab 2.0 database and regional seismic tomography. Locally thickened crust from the Hikurangi plateau, a large igneous province actively being subducted, is also included in the slab geometry. To simulate realistic deformation, we use a composite viscoplastic rheology, including the effects of brittle failure, low-temperature plasticity, and high-temperature creep. Phase transitions at depths of 410-km and 660-km produce density discontinuities which more accurately capture negative buoyancy forces driving subduction. Driven purely by slab pull forces, the models exhibit corner flow in the mantle wedge and reproduce plate speeds comparable to relative plate speeds observed between the Pacific and Australian plates. These results represent the first fully dynamic 3D viscoplastic subduction simulations performed for the Hikurangi-Kermadec system. Future work will be to include fluid transport in tandem with slab hydration/dehydration reactions to simulate melting in the mantle wedge.



Top figure: 3-Dimensional isosurface of the slab coloured by temperature. Vectors are coloured by velocity magnitude and show flow direction in the upper mantle. Bottom figure: 2-Dimensional cross section through the North Island of New Zealand perpendicular to the strike of the trench. Fields are the same as the top figure. Variable lithosphere thickness is visible in both overriding and subducting lithospheres.

## **Cross-Time-Scale Dynamics of Subduction Seismic Cycles: From Megathrust Ruptures to Large-Scale Plate Motions**

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Subduction zones host great megathrust earthquakes. The spatiotemporal variability of these earthquakes is thought to be intimately coupled to plate tectonics and underlying mantle dynamics. However, it is challenging to incorporate viscous mantle convection and elastic earthquake rupture in one model to bridge their substantially different time scales. Here we develop a 2D self-consistent subduction zone model using the finite element code Underworld, aiming at closing the gap between large-scale, long-term geodynamical control and local-scale, short-term seismic cycles. The model employs a nonlinear viscoelastoplastic rheology to simulate the long-term behavior of lithosphere and upper mantle. Negative buoyancy from a denser slab drives motions of tectonic plates. A thin shear zone is implemented between subducting and overriding plates to mimic the fault interface, with a velocity-weakening rate-and-state friction law to trigger spontaneous slip instability and generate earthquake sequences. By taking adaptive time steps from milliseconds to ten years, it reproduces multiscale processes at different stages of seismic cycles.

We successfully model multiple subduction seismic cycles in computations. In the interseismic period, the subducting plate moves at several centimeters per year. When an earthquake occurs, coseismic ruptures initiate in the seismogenic zone and propagate downward along the fault, with slip velocity increasing by ten orders of magnitude in a short time. During the main thrust event, the subducting plate reaches a dramatically high convergence rate near the trench, while the far end preserves the long-term horizontal velocity. The overriding plate, which was originally locked, gets decoupled and jumps to the opposite direction. The long-term behavior of plate motion is restored in the postseismic relaxation over tens of years. We also observe from the model that stress accumulates near the fault zone as two plates become coupled in interseismic periods and rapidly releases when earthquakes occur. Moreover, cumulative displacement measurements along the surface are consistent with geodetic observations. The multiscale model demonstrates the capacity of simultane- ously capturing short-time-scale and long-time-scale features in multiple seismic cycles, and the potential in investigating geodynamical underpinnings of great megathrust earthquake occurrence.
### Exploring the Cascadia slab structure coupling 3D thermomechanical and CPO modeling

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The Cascadia Subduction Zone is characterized by young subducting lithosphere, its isolation from other subducting systems, and its ability to produce megathrust earthquakes (M > 9.0) and devastating tsunamis. Due to its high potential hazard and risk, it is also a well-studied subduction zone where modern, diverse and detailed observational datasets are available through the USGS and initiatives like GeoPrisms and EarthScope. These datasets include high quality GPS, onshore and offshore geophysical imaging, geochemical and seismic anisotropy data. These datasets present an opportunity to gain insight into slab structure, tectonic evolution, and present-day seismic hazards. Still, many questions remain about the physical processes that can self-consistently explain all the observations, and better estimate seismic hazards. For example, geologic and geophysical data suggest that there may be one or two prominent slab gaps or tears, while tomographic data does not fully constrain the depth extent of the slab. Furthermore, the overriding plate is composed of several different terranes and contain numerous active and slowly moving faults, complicating efforts to accurately constrain variations in present-day stress and deformation rates.

In this study we test whether comparison of observations to model predictions can distinguish between different slab geometries for the Cascadia Subduction Zone. To this end, we have created regional 3D geodynamic models of Cascadia including the slab based on the Slab 2.0 dataset. The model setup is built with the Geodynamic World Builder, and the models are run using the mantle convection and lithospheric dynamics code ASPECT. During the evolution of these models we track the development of the CPO (Crystal Preferred Orientation), so we can compare it against seismic anisotropy data of the region. Our presentation will focus on the preliminary results of these models and demonstrate workflows for linking the model results to surface tectonics. We will also highlight some of the development in ASPECT and the Geodynamic World Builder that was needed to achieve these results.



Top view of the model of the Cascadian subduction zone. The colors on the model show viscosity, and the arrow and their colors show velocity in the lithosphere. The model is 800km deep.

## Investigating the factors controlling trench migration rates in narrow subduction zones

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Subduction processes are thought to be the main drivers of plate motion and mantle flow. Thus, much effort has been put to understand subduction dynamics through numerical and analog modelling. The large variety of subduction zones observed in nature highlights the complexity of these processes, which are influenced by a wide variety of factors including the slab density and length, the mantle rheology and/or the overriding plate strength. Previous studies have found that slab width plays an important role on the trench migration velocity, which decreases with increasing slab widths (e.g., Schellart et al., 2007). However, other modelling studies have shown that this trend is not followed for narrow subduction zones, concluding that there is a finite slab width for which the trench retreat velocity is maximum (e.g., Stegman et al., 2006). The subduction zone width at which the trench velocity peaks varies depending on the published works (e.g., Stegman et al., 2006; Strak and Schellart, 2014), suggesting a dependence of this behaviour on different factors that are still poorly understood. This study aims at identifying which are the factors that exert a dominant control on trench retreating velocity in narrow subduction zones (i.e. slab width < 1000 km). We perform 3D numerical modelling, which includes subducting, overriding and lateral plates (Fig. 1), to systematically evaluate the effect of slab width, strength of coupling with the lateral plate, and overriding plate thickness.

Contrary to what occurs for moderate to wide subduction zones, we obtain that slab width has little influence on trench retreat velocity for narrow subduction zones. This is in agreement with observations in natural narrow subduction zones showing no direct relation between slab width and trench migration velocity. Instead, the major influence is exerted by the thickness of the overriding plate. Finally, the strength of coupling with the lateral plate is also shown to have little influence on trench retreat velocity, although the slab width exhibiting the maximum retreat velocity slightly increases as this coupling strengthens.



Figure 1: Schematic illustration of the 3-D model setup (2000x800x660 km) and boundary conditions

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# Boundary condition controls on flat slab subduction and intraplate deformation

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Plate boundary conditions (i.e., end loading vs basal traction) that drive intraplate deformation along inherited weaknesses are poorly studied by geodynamic modelling. We focus on intraplate deformation of the Laramide orogeny that occurred up to 1000 km from the subduction front in central North America during the Upper Cretaceous to Paleogene. The most accepted driving mechanism for the Laramide orogeny is a flat-slab subduction event. Therefore, our aim is to recreate a flat-slab subduction event by subducting a buoyant portion of oceanic crust (oceanic plateau) and to investigate i) how stresses are affected by movement of the overriding plate. In the first case a converging velocity is assigned only to the down-going slab, allowing quantitative and qualitative assessment of stress transmission through the plate interface. In the second example a convergence velocity is prescribed to both the down-going slab and the overriding plate. In both cases an inherited weakness is placed approximately 600 km inboard from the subduction front and the orientation and magnitude of the minimum and maximum principal stresses are calculated and plotted.

We present the preliminary results from geodynamic modeling of the two scenarios to understand how differing flat-slab subduction boundary conditions affect force transmission into the overriding plate and how these forces affect intraplate inherited weaknesses. We show that maximum principal stresses can be transmitted far (over 1000 km) into the overriding plate interior, that up to 40% of stress in the overriding plate can be transmitted across the plate boundary from the down-going slab, and that intraplate deformation 1000 km from the plate boundary does not require a long flat-slab segment.

## Geodynamic constraints on ophiolite emplacement

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Ophiolites are the part of the oceanic crust and upper mantle and have been extensively studied for more than half a century (Gass 1968, Moores & Vine 1971, Coleman 1977). And ophiolites gave a lot of understanding to fundamental processes in oceanic crust and lithosphere in general. (Burg, 2017). Although it gave a lot, there is no consensus on how them ophiolites have been formed. Answering that question might help reconstruct the history of tectonic activity in that region, especially in the zone with small ocean basins like in Troodos. Earlier authors (like Cloos and etc) derived that subduction initiation is driven by the negative buoyancy of colder lithosphere. However, it is based on isostasy analysis, which means the lithosphere has no shear strength and is only supported by floating forces on the asthenosphere. That gives an additional constraint that the lithosphere must have been young and hot to be emplaced on top of continental crust before it becomes heavier.

Another problem is that ophiolites are different between each other in different regions. There are 'Tethyan (Mediterranean)' that are obducted over passive continental margins and 'Cordilleran (Pacific)' that are incorporated into accretionary wedges. Moores (1982)

Studying a vertical profile also raises a range of questions. Study of metamorphic sole from Semail Ophiolite indicates that it has experienced high temperature and has an inverted temperature gradient towards the deeper part of the sole, where it ends with almost non-metamorphosed rocks.

In comparison with subduction and rifting, obduction is a relatively rare tectonic scenario that makes studying obduction harder. For example, having subduction occurrences in different conditions, which we can see on the margins of different tectonic plates, gives us different angles to look at the result of subduction and eventually have a better understanding of what happened.

Some recent studies with numerical models (Duretz , 2016) create a two stage process of the subduction and exhumation to emplace an ophiolite. Duretz provides a study where he indicates that 350-400 km bulk shortening gives best fit for PT conditions of metamorphosed margin. It gives a possible explanation of a rare occasion of ophiolites, that it needs a particularly restrictive set of necessary boundary conditions. It was noted that presence of thermal anomaly is key to match high temperature that experienced metamorphic sole. Thermal anomaly allows to have a younger (less than 10 Ma) oceanic plate, which can be less rigid and, particularly in obduction case, make a more favourable behaviour to be emplaced on top of continental part.

In this work we performed self-consistent geodynamic models with variable densities, that are derived for specific pressure and temperature. With respect to density, the buoyancy state of tectonic plates is also dynamic. We found that the obduction process is sensitive to all mentioned above parameters and will try to find the best set of parameters with respect to first order geological constraints.

As a result, we present a set of models where we can observe successful emplacement of part of the oceanic crust on top of continental crust. Model fits with known time constraints and mechanical parameters and can help answer the question of forming ophiolites. State of the art thermomechanical code LaMEM with visco-elasto-plastic rheology also reveal that shear heating also takes place in time of forming of ophiolites and might influence peculiar inverted metamorphic gradient in metamorphic sole.

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## Numerical model of slab pull related continental breakup

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The Earth records a multitude of continental fragmentation events ranging from the global dismantling of super-continents (e.g. Columbia, Rodinia, Pangea, Gondwana) to the formation of micro-continents on a regional scale (e.g. the Seychelles, the Jan Mayen, the Palawan Island, the Cimmerian blocks). Continental breakup occurs when the extensional stress exceeds the strength of the lithosphere, and several mechanisms have been proposed to explain the origin of this extensional stress regime. One of the most studied is the plume-induced continental breakup. However, previous numerical studies have suggested that mantle upwelling does not provide sufficient forces to breakup a continental plate in the absence of far-field extensional forces or other weakening mechanisms such as the injection of magmatic dykes. While slab pull is known to be the driving force of plate tectonics and slab roll back has already been identified as responsible for back-arc basin formation, very few studies have investigated the slab pull related continental breakup mechanism.

Here we present a 2D thermo-mechanical regional-scale model of ridge-free subduction with slab pull evolving self-consistently during slab sinking in order to understand how, when and where slab pull can lead to continental break up. Our numerical simulations reveal that the marked increase of slab pull induced by the crossing of the 410 km phase transition may lead to continental breakup within the lower plate after the mid-oceanic ridge subduction. We show that the relative motion between the tectonic plate and the underlying mantle strongly controls the localisation of the deformation. If the horizontal displacement of the lower plate continent significantly differs from that of the mantle below, the basal shear between the lithosphere and the asthenosphere prevents the development of the necking instability and the extensional deformation remains distributed all along the continent. On the contrary, if the continent moves at the same velocity as the mantle, deformation eventually localises near the passive margin and results in the formation of a micro-continent drifting towards the subduction zone.

In the light of this study, the slab pull appears as a major contributor to continental breakup and might be involved into the formation of several micro-continents, such as observed for the Cimmerian blocks during the Permian and for the opening of the South China Sea during the Oligocene.



Figure 1: Snapshots of our model of slab pull related continental breakup.

# Progressive weakening within the overriding plate during dual inward dipping subduction

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Dual inward dipping subduction often produces complex deformation patterns in the overriding plate. However, the geodynamic process of how dual inward dipping subduction relates to this deformation is still poorly understood. Here we apply a composite viscosity, incorporating dislocation creep, diffusion creep, yielding and Peierls creep, in 2-D thermo-mechanical numerical modelling to investigate how dual inward dipping subduction modifies the rheological structure of the overriding plate.

Three variables on the plate sizes are investigated to understand their roles in controlling the maximum degree of weakening in the overriding plate. We find that the initial length and thickness of the overriding plate are negatively correlated with the magnitude of viscosity reduction, while the initial thickness of the subducting plate positively relates to the magnitude of viscosity reduction. The progressive weakening can result in a variety of stretching states ranging from 1) little or no lithosphere thinning and extension, to 2) limited thermal lithosphere thinning, and 3) localised rifting followed by spreading extension. Compared with single-sided subduction, dual inward dipping subduction further reduces the magnitude of viscosity of the overriding plate. It does this by creating a dynamic fixed boundary condition for the overriding plate, and forming a stronger upwelling mantle flow which induces progressive weakening in the overriding plate.

Further investigation on the evolution of the dominant deformation mechanism shows that dislocation and yielding contribute most to induce rifting and spreading extension, which initiate from the bottom of the overriding plate (Figure 1). The progressive weakening is mainly driven by the ever-increasing strain rate, which is also a precondition for initiating a positive feedback weakening loop that incorporates viscosity reduction, strain localisation, thermal lithosphere thinning and formation of new plate boundaries.



Figure 1. Scatter plots of the dominant deformation mechanism along the midline of the overriding plate (5000 km away from both side boundaries), i.e., the main necking region. (a) The temporal path of each dominant deformation mechanism (DDM) is plotted on a phase diagram, where the background contour map represents the magnitude of viscosity. The phase diagram is divided by the white dashed lines into four domains based on the calculation of which component deformation mechanism yields the minimum viscosity at the given strain rate, temperature and depth. (b) The scatter plot evolution of the dominant deformation mechanism that yields the minimum viscosity (MVDDM) throughout the midline of the overriding plate.

## A Simple Force Balance Model of Subduction Initiation

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The initiation and development of subduction zones are associated with substantial stress changes both within plates and at plate boundaries. We start from a simple analytical model based on the force balance equation of a subduction zone cross section and validate it with numerical calculations of the highly non-linear, coupled thermo-mechanical system. We extend the analysis from a cross section to 2.5D, a sliced 3D geometry with an along strike dimension degree of freedom, to explore the role of strike slip motion in subduction initiation. Finally, we compute a case study of Puysegur subduction in 3D to investigate the stress evolution of an incipient subduction zone. In the analytical model, we quantify the role of each component of the force balance, including slab pull, inter-plate friction, plate bending, and basal traction, on the stress state of a subducting plate. Based on the numerical and analytical models, we discuss the evolution of plate curvature, the role of plastic yielding and elasticity, and how different factors affect the timing of subduction initiation. We demonstrate with the presence of plastic yielding for a plate of thickness, *H*, that the bending force is proportional to  $H^2$ , instead of  $H^3$  as previously thought. Although elasticity increases the force required to nucleate subduction it does not substantially change the total work required to initiate a subduction zone when the yield stress is small [e.g. leq 300Mpa]. Plate convergence and weakening during nucleation are the dominant factors influencing the force balance, and 200 km of plate convergence is typically required to bring a nascent subduction zone into a self-sustaining state. We show that strike slip motion effectively accelerates the weakening process, reduces the resistance at a plate boundary and make subduction initiation easier. A strain partitioning arises during the transfer of strike slip from the strike slip fault to the oblique subduction zone. In the 3D model, the plate stress from numerical models experiences a transition from compression into extension, consistent with the analytical model. From northern to southern Puysegur, the subduction zone experiences different phase of the compression-extension stress transition, indicating a propagation of subduction initiation along strike.

## Mantle exhumation and continental fragments formation in backarc basins

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Back-arc basins often present multiple spreading centres that form one after the other (e.g. Mariana subduction zone), propagate and rotate (e.g., Lau Basin) following trench retreat. In some cases, rift jumps can create continental fragments or microcontinents (e.g., Coral Sea, Central Mediterranean, Scotia Sea) and/or cause mantle exhumation and intrusions of magma bodies that are emplaced discontinuously in time and space (e.g., Tyrrhenian Sea). All these features reveal a picture of a back-arc basin that is much more complex than that of seafloor spreading at mid-ocean ridges. Importantly, the processes controlling rift jumps and mantle exhumation are still not fully understood, but they are certainly related to the dynamics of subduction and mantle flow.

In this work, we show how episodic trench retreat shapes the morphology of back-arc basins and can produce rift jumps. We use the finite element code ASPECT to model the rifting of continental lithosphere in 2D with boundary conditions that simulate the asymmetric type of extension caused by the trench retreat. We perform a parametric study in which we systematically vary the duration of different extensional phases, simulating episodes of trench retreat. Our results show that when extension is continuous, continental break-up occurs and a spreading centre, similar to a mid-ocean ridge, develops. On the other hand, in models with multiple extensional phases, ridge jumps consistently occur and are often associated with mantle exhumation between the old and the new spreading ridge. In some cases, continental fragments are separated from the main continent and end up being surrounded by oceanic basins. These results are in good agreement with what observed in many back-arc basins today. Timing and length of ridge jumps depend on rheological properties of the lithosphere, but, importantly, we show that the resulting back-arc basin morphology is controlled by the duration of the different stages of extension.



Different resulting structures of back-arc basins depending on the time of the first extensional phase; (a) the continental margin on the left of the basin is much more stretched than its conjugate margin on the right, (b) formation of a continental fragment bounded between two oceanic basins and exhumed mantle, and (c) intra-oceanic ridge jump.

# High thermal conductivity of stishovite promotes rapid warming of a sinking slab in Earth's mantle

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Here we present thermal conductivity measurements on stishovite. We found that *Lambda*St at ambient conditions is extremely high: 80 W/m K. Therefore, the aggregate thermal conductivity of the oceanic crust is higher than the one of the lithospheric slab.

We designed a numerical model with a vertically sinking slab composed by two layers: the lithosphere and the crust. We solved the 1D heat diffusion equation with the implicit FD method. We run 8 different scenarios in which we changed the fraction of stishovite in the crust. Our models reveal that St-rich crust will warm up much faster than St-rich poor crust. A warmer crust will experience: a) downward deflection of the post-garnet phase transition; b) enhanced buoyancy; c) reduced viscosity.

A hypothesis can be formulated (Figure 1): St-rich lenses in the crust can induce the fast warming of the surrounding rocks. These lenses of unreacted crust may detach from the rest of the slab and stagnate in the mantle transition zone (MTZ). The cold and reacted regions of the crust, instead, will continue their journey into the LM. The presence of oceanic crust in both MTZ and LM is suggested by geophysical observations.



Figure 1. Potential mechanism to explain the presence of metabasaltic crust in the MTZ and in the LM.

## Extension and inversion of rotational and oblique rifts, as inferred from 3D coupled thermo-mechanical and surface processes models

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Continental extension is often oblique, resulting in rotational rifts with characteristic V-shaped basins, oblique transtensional structures and along-strike variations in the overall lithospheric structures. Inherited crustal or mantle heterogenities exert a first-order control on the structural style of extension and subsequent basin inversion, and lead to different uplift-subsidence rates in the modeled basins and orogens.

In this study, we conducted a series of 3D numerical experiments to simulate the successive stages of rotational and oblique rifting and subsequent basin inversion in order to understand the resulting strain partitioning and lateral variations, while also tackling the coupling between tectonics, mantle melting and the surface processes. We applied the coupled I3ELVIS-FDSPM numerical code (Gerya 2015, Munch et al. 2022), that is based on staggered finite differences and marker-in-cell techniques, solves the mass, momentum and energy conservation equations for incompressible media, and also takes into account simplified melting processes and erosion-sedimentation by diffusion.

The modeling results are compared to observation data from several Mediterranean back-arc basins. In the Tyrrhenian, Pannonian and Alboran Basins, temporal variations of different plate convergence rates, slab retreat velocities and rotational plate movements lead to rotational/oblique extensional basin formation, which recently changed to structural inversion. In fossil rifts, such as the Pyrenees and Great Caucasus, the inversion has already reached the mature orogeny phase, where high strain-rate convergence has ultimately overprinted the former basin structure. The study was supported by the 134 873 OTKA research fund.

# Complex phase transitions and seismogenic stresses in the Tonga subduction region

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The Tonga-Kermadec-Hikurangi subduction zone forms a compact and one of the most complex plate tectonics systems on planet Earth. The tectonism in the Southwest Pacific region started in the Late Cretaceous (i.e. approx. 100 Ma ago). The onset of subduction of the Pacific plate below the Australian plate along the Tonga-Kermadec-Hikurangi subduction zone still remains enigmatic and a subject of scientific debate. According to previous research a wide range of 30-85 Ma [e.g. van de Lagemaat et al., 2018] was suggested for the subduction initiation in this region. Nowadays, the Pacific plate is subducting under the Australian plate at the Tonga-Kermadec-Hikurangi subduction boundary moving west-northwestward at a velocity of approximatelly 5 - 11 cm/yr [Schellart and Spakman, 2012].

Focal mechanisms of deep earthquakes in the transition zone usually show down-dip compressional stresses which are typical for slabs at these depths due to the resistance to penetration into the lower mantle. The Tonga slab seems to be special in this regard. Fukao et al. [2014] observed a set of unusually deep earthquakes at 680 km depths to exhibit focal mechanisms with vertical tension and horizontal compression. Such rotation of compressional stress axes toward the horizontal is most probably connected with the forces exerted by the phase transitions and viscous resistance of the lower mantle. They could be caused by various effects: bending of the slab in the transition zone, viscous coupling between the slab and the lower mantle when the bent portion of the slab is driven sideways, interplay between the positive petrological buoyancy and negative thermal buoyancy of the slab above and under the 660 km phase transition. The phase transitions in this exceptionally old and cold slab are probably affected by recently reported complicated phase transformation of ringwoodite to bridgmanite through akimotoite. In this study we employ numerical modelling to test the above mentioned mechanisms and their effect on possible stress rotation.

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# Plate interaction and the role of the flat-slab subduction in the Central Andes

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Most The convergent western South American margin hosts one of the longest non-collisional orogenic belts on Earth. With more than 7000 km in length, the Andes straddle the western margin and constitute a subduction orogen with latitudinal differences in volcanic activity, deformation styles, amounts of shortening and differences in subduction angles. From the southern Central Andes where the Andean Plateau terminates at approximately 27°S to the Southern Andes at about 33°S, the subduction angle of the oceanic Nazca plate changes from steep to flat. This sector of the subducting plate is also known as the Pampean flat slab. The change in subduction angle has been attributed to the southward migration of the Juan Fernandez hot spot ridge beneath the continental South American plate. The role of the passage of the Pampean flat slab in the contemporaneous acceleration of the shortening rate from 21°S at the latitude of the Andean Plateau at 35 Ma to its present latitude at 33°S is strongly debated. Besides, most of the growth of the Central Andes, including the formation of the Andean Plateau (Altiplano-Puna Plateau), mainly occurred during two shortening pulses at 15 Ma and 7 Ma, suggesting a complex interplay between subduction dynamics and its interaction with the overriding plate.

To investigate the role of the subducting flat slab in upper-plate deformation, we developed two models with the FEM geodynamic code ASPECT: (i) A 3D data-driven model incorporating the current Pampean flat-slab configuration (26-42°S) to assess its role in the localization of the deformation; and (ii) a series of high/resolution 2D self-consistent E-W-oriented subduction models at the latitude of the Altiplano-Puna Plateau (21°S), which includes a flat-subduction episode at 35 Ma and tracks the evolution of lithospheric shortening.

We propose that initial crustal contraction in the foreland of the continental South American plate foreland occured during shallowing of the slab. Furthermore, we suggest that the pulses of increase in shortening rate in the Central Andes are a consequence of the decrease in absolute westward motion of the South American plate during the last 25 million years, which caused the anchored slab in the lower mantle to buckle in the mantle transition zone at 15 and 7 Ma. At the

start of each buckling cycle, the slab steepened and the trench resisted. Therefore, the difference in velocity between the overriding plate and the trench was accomodated by shortening in the orogen, which was previously weakened by removing lithospheric mantle due to the passage of the flat slab.



Figure 1. 3D data-driven model of the southern Central Andes.

# Determination of the structure and rheology of a fluid allowing self-consistent subduction during convection in the laboratory

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Subduction of the lithosphere is a main feature of Earth's mantle plate tectonics and convective dynamics. To date, we have found only one fluid able to produce in the laboratory self-consistent subduction during convection : colloids of silica nanoparticles (Ludox ®) [1]. The latter provides a large diversity of regimes depending on the nanoparticles volume fraction and the history of the material. From fluid to solid right through to gel, many structures can be observed [2]. It is important to identify which conditions are necessary to generate subduction.

Convection in this colloids can have a thermal origin (when the tank is heated from below) and/or a solutal origin (when Ludox®'s water evaporates). Regardless of its nature, convection creates heat and mass transfers which affect the fluid structure's organisation and lead to concentration gradients. These concentration gradients produce different fluid characteristics (Newtonian or shear-thinning, yield stress. . . ), which in return, influence the convective patterns. Finally, it also leads to a stratified system with a denser and stiffer skin on the surface (figure 1). This stratified system allows episodes of self-consistent subduction : the skin formed on the surface breaks and sinks into the less-viscous fluid bellow. With the help of thermal analysis (Differential Scanning Calorimetry, DSC, and Thermogravimetric Analysis, TGA) and Small-Angle Neutron Scattering (SANS), [3], we can evaluate volume fractions and fluid texture (e.g. typical size of ag- gregates, formation of a more or less compact skeleton. . . ) for the different states present in the convective system (liquid, paste, skin and subducted skin). Then, these measures can be linked to the fluid's rheology. Thus, we can determine the rheological conditions for which the convective system is able to trigger subduction.



caption

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# Shallow and deep tectonic structures of the Zagros collision zone and surroundings

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The Zagros collisional zone, formed from the collision of the northern margin of the Arabian platform with the microplates of central Iran, extends from the Turkish–Iranian border to the NW, to the Makran area in the SE. It is composed of different parallel tectonic features from southwest to northeast: the Zagros Fold and Thrust Belt (ZFTB), the Sanandaj–Sirjan Metamorphic Zone (SSZ), and the Urumieh–Dokhtar Magmatic Assemblage (UDMA). Present-day kinematics indicates a northward motion of the Arabian plate relative to Eurasia of  $22 \pm 2 \text{ mm yr}^{-1}$  (e.g., Khorrami et al., 2019). The geodynamic setting of the area is quite complex and several issues concerning the continuity and inclination of the subducted slab have not been fully addressed by the previous studies.

In the frame of the project PRIN 2017 (Intraplate deformation, magmatism and topographic evolution of a diffuse collisional belt: Insights into the geodynamics of the Arabia-Eurasia collisional zones), we analyze global (Schaeffer and Lebedev, 2013) and regional (Koulakov et al., 2011) seismic tomography models and convert their absolute velocities in temperature, assuming a composition representative of a Phanerozoic and Proterozoic mantle, characterizing Central Iran and Zagros collision zone, respectively. To this purpose, we use Perple\_X (Conolly, 2005) that computes physical properties for a given mineralogical model, expressed by the main mantle oxides. We also compare the results obtained with the seismicity distribution (1976-2022, M>=2.5, https://www.usgs.gov/programs/earthquake-hazards/national-earthquake-information-center-neic) and the depth of the Curie point (Li et al., 2019).

We observe that most of seismicity occurs in the thick crust (> 50 km) and is located in the ZFTB, while the SSZ is mostly aseismic. Such a difference between these tectonic features can be ascribed to the cold Arabian slab that underlies the crust of the ZFTB, favouring a brittle behaviour and seismicity. On the other hand, the absence of the Arabian lithosphere beneath the SSZ, due to the steepening or even break-off of the slab, can likely induce ductile conditions in the overlying crust, preventing earthquakes nucleation. Indeed, the abrupt decrease of seismicity is accompanied by a sharp decrease of the Curie depth and upper mantle velocity, as well as a transition to a smoother topography. More to the north, beneath Central Iran, the lithosphere is quite thin (< 100 km), crustal thickness reduces to 40 km, and topography is low and flat, as effect of the lithospheric delamination occurred in the Eocene, before the continental collision.

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# Three-dimensionality of Slab Thermal structure within Dynamic Subduction Models

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The thermal structure of subduction zones regulates important processes such as dehydration reactions along the downgoing slab, seismicity, and arc volcanism. Previous two-dimensional modeling studies suggest that slab temperatures evolve over a few Myr (e.g., Holt and Condit, 2021), making it crucial to study time-dependent subduction models. Moreover, three-dimensional studies (e.g., Kincaid and Griffiths, 2003) suggest that temperatures vary along-strike, which suggests that 3-D effects have important consequences on slab temperatures. Given these two sources of variability, we study 3-D dynamic models, to understand how the along-strike variability evolves throughout the subduction process. We model three-dimensional, dynamic subduction using the ASPECT finite element code (Kronbichler et al., 2012; Bangerth et al., 2021). We focus on the difference between thermal conditions at the plate edge vs at the plate center, and on the effect of both plate width (1000 vs 2000 km vs. Infinite width/2-D) and trench motion (free vs fixed overriding plates). Our models show that, for both fixed and free overriding plate cases and all plate widths, the edge of the plate is warmer than the center during the early stages of subduction (by  $\geq$  30°C) while, during mature subduction, the center becomes warmer than the edge (by  $\geq$  32°C). These trends are primarily a result of the spatio-temporal variability in poloidal flow, toroidal flow, and the depth of decoupling, with flow pattern effects being particularly pronounced in the free-overriding plate case. During mature subduction, our study predicts lower magnitudes for the along-strike temperature variation than those estimated in the laboratory models of Kincaid and Griffiths (2003) ( $\geq$  120 °C), but the along-strike sense of temperature variation is comparable. Given the along-strike time-dependent variability, which is likely reflected in spatio-temporal variations in arc magmatism and slab dehydration, our models suggest a 3-D, dynamic setting is crucial to understand the thermal structure of subduction zones.

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# The influence of far-field mantle density anomalies on subduction dynamics

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Density anomalies are distributed throughout the mantle, as can be inferred from seismic tomography, and are typically attributed to mantle temperature variations. At subduction zones, the forces exerted on slabs, and hence subduction properties (e.g., dips, convergence rates), can be affected by such anomalies due to the mantle flow they induce. Despite this, most numerical subduction modeling studies limit subduction to within a regional box and so neglect these effects. Here, we quantify how subduction dynamics is affected by distant mantle anomalies by investigating the influence of density anomaly location, size, and amplitude within idealized global models. These models are in 2-D (i.e., a spherical annulus) and were developed using the ASPECT finite element code. In agreement with other recent work, our preliminary results show that far-field density anomalies can have a significant effect on subduction dynamics. Initially focusing on convergence rate, we find that the larger the anomaly, or the closer it is to the slab, the larger the impact on convergence rate. A lighter anomaly (e.g., a plume) increases the convergence rate; A heavier anomaly (e.g., a slab fragment) reduces the convergence rate. For example, a 200 km size anomaly with 100 kg/m<sup>3</sup> greater density than the mantle decreases rates by 3 cm/yr for anomalies within 30 degrees of the slab. Future work will include more detailed analysis of the subduction zone (e.g., the pressure forces), extending models to 3-D, and "realistically"-shaped anomalies based on tomography.

## Dynamics of upper and lower mantle subduction and its effects on the amplitude and pattern of mantle flow.

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Numerical models of mantle convection are constrained by reconstructed and active plate motions, geochemical composition and evolution of Earth's interior or seismological observations of modern mantle structure. However, these constraints still allow for a widely varying behavior of mantle flow, as numerical models using similar constraints defend highly mobile whole mantle convection, layered convection, or hybrid variants of these. As a result, predictions about mantle structure also vary greatly, predicting a well-mixed mantle or a strongly heterogeneous mantle possibly containing primordial mantle material.

Subducting plates all over the globe and in the geologic past have a variety of different velocities and morphologies in the upper mantle while that mantle has basically the same structure everywhere on the planet. A new kinematic constraint (vd Meer et al. 2018) shows that after subduction these slabs tend to sink with similar velocities in the Lower Mantle, a magnitude slower than plate motion (10-15 mm/a), despite their different shapes and sizes. We model subduction in a 2D-spherical shell to accommodate subduction with known plate motions while keeping sinking rates tailored to the new kinematic constraint by changing the rheologic properties of the lower mantle. As a result, we show that mantle convection might occur on a more local scale and with lower magnitudes than previously shown, leading to limited mixing and the possible preservation of mantle heterogeneities over at least a billion years.

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# How subduction dynamics, crustal tectonics and surface processes are reflected in orogenic plateaus?

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Mountain belts are major tectonic features on Earth that reflect the relation between plate convergence and crustal thickening, small or large-scale subduction and mantle convection effects as well as surface processes, namely erosion and sedimentation. The Himalaya and Tibetan Plateau built upon uniquely high plate convergence velocity have been regarded as presentative of mantle orogeny, often considered to be associated with large scale mantle convection (e.g., Faccenna et al. 2013).

Since India collided with Asia about from ca. 55 Ma, the rise of the Tibetan plateau likely occurred in three main successive stages, leading to specific uplift patterns and crustal tectonics (Tapponnier, 2001). But how such topography is supported by crustal, lithospheric and deep mantle effects remains unclear. We simulate the formation of the Himalaya and Tibetan Plateau, trying to understand the spatial and temporal evolution of orogenic plateau formation and its connection to upper and lower crustal deformation, lithospheric mantle delamination and deep subduction dynamics.

To this aim, we use 2D numerical modeling with I2ELVIS code (Gerya & Yuen, 2007) to simulate oceanic and subsequent continental subduction and collision associated with various tectonic and magmatic processes. Tectonic plates are represented by two continents separated by a ca. 700 km wide oceanic lithosphere. We present preliminary results on the influence of different subduction velocities, plate rheology and different intensity of surface processes for different geodynamic regimes of orogeny and plateau formation.

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# How does an arc influence a back-arc extension: insights from 2D numerical modeling

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A back-arc basin is located at the rear of an arc in a subduction system. Even though they are all termed as 'back-arc' basins, most of them are formed by splitting a volcanic island arc, which results in a remnant arc on the other side of the basin. The factors that influence the location of the extension on the overriding plate (OP) are not fully understood.

We ran 2D thermo-mechanical models of a subduction zone based on the set-up of Garel et al. (2014). In addition, a hot region was introduced on the OP to simulate the role of an arc on the back-arc extension. The reference model (RM) without the hot region shows a slightly thinned OP 750km away from the trench. We tested three parameters relevant to the hot region based on the RM: the distance from the hot region centre to the trench (Distance), the width of the hot region (Width), and the increased temperature of the hot region centre ( $\Delta$ T). The models show three modes of back-arc extension: (a) only thinning the same as RM, but no back-arc extension on the OP (NE); (b) back-arc extension occurs far away (around 750km from the trench) from the hot region on the OP (EF); (c) back-arc extension at the hot region (EH), there is slab detachment in some models (EH-D), but not in others. The transitions from mode (a) NE to (b) EF, to (c) EH occur with increasing Distance, Width, and  $\Delta$ T. While the slab detachment occurs only with increasing  $\Delta$ T.

We noticed that the SP sinks more rapidly and the trench retreat rate increases at the same time when the hot region is heated and weakened (the rheology is temperature-dependent) more by increasing  $\Delta T$  or Width, which is corresponding to a stronger mantle wedge flow driving the extension on the OP. As the hot region is made weaker, this region is more likely to breakup, and therefore this leads to the migration of the spreading centre from the location 750km away from the trench (EF) to the hot region itself (EH). It can be seen that  $\Delta T$  plays the most significant role on the back-arc extension in our models.



Figure. Snapshots showing the viscosity field of reference model (RM) and the different modes of back-arc extension in different models.

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## Rheology of the deep subduction interface and its role in influencing short- term seismic style and long-term subduction dynamics

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I'll be presenting work my students, colleagues and I have been doing to better understand the mechanical behavior of subduction interface shear zones over both the short timescales of seismic behavior and the long timescales of geodynamic plate motions. I will use observations from both the field and lab to demonstrate that interface rheology is highly sensitive to the types of materials (e.g. sediment vs. mafic rocks) that are subducted to depth. In considering short timescales, I'll show how mixed lithology interfaces generate heterogeneous shear zones that may produce seismic behaviors that resemble episodic tremor and slow slip. In considering longer timescales, I'll demonstrate how the viscosity contrast between different subducted rock types affects subduction plate speeds, thus setting up potential connections between Earth's interior dynamics and surface processes that influence sediment delivery to the seafloor.

## **Recent Progress in the Experimental (and Theoretical) Study on Plastic Deformation Under Deep Mantle Conditions**

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We will report some of the recent results on plastic deformation of minerals under the deep mantle conditions. Most plastic deformation in Earth occurs below the lithosphere where pressure exceeds 2-3 GPa. Quantitative deformation experiments under these conditions were difficult if one uses conventional equipment such as the Paterson apparatus (this apparatus works below 0.5 GPa). During the last 20 years, a major breakthrough in deformation experiments has been made using the synchrotron X-ray (mostly done by Don Weidner). In combination with new deformation apparatus such as RDA (rotational Drickamer apparatus) or DDIA (deformation DIA), quantitative data on deformation have now been obtained to P to 30 GPa and T to 2000 K.

These new techniques allow us to characterize the stress distribution in deforming minerals including stresses on different co-existing minerals as well as stresses of the same mineral but on grains with different crystallographic orientations. By monitoring the stress evolution as a function of time (strain), we can now characterize the evolution of strength of mineral aggregates (at high P and T). Using a theory of radial X-ray diffraction (Karato, 2009), these results allow us (i) to infer deformation mechanisms (diffusion versus dislocation creep), (ii) to characterize the evolution of the slip system that controls the strength of an aggregate, as well as (iii) to characterize the contrasting strength of co-existing minerals and the evolution of stress-strain partitioning in the two-phase mixtures.

Some examples on the results on the bridgmanite-ferropericlase mixture, fine-grained ringwoodite and olivine aggregates will be shown. In addition to a marked difference in creep strength between bridgmanite and ferropericlase and weak creep strength in fine-grained ringwoodite, we will report new results on transient creep in olivine aggregates where the role of evolving inter-granular strain (stress) partitioning is demonstrated. Some geodynamic implications will be discussed including the possible mechanisms of shear localization and transient creep.

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#### **\*** Invited speaker

## How Microscopic Crystalline Defects Control the Motion of Tectonic Plates

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The modes of mantle convection and its tectonic manifestation differ from one rocky planet to another, but the physics that govern it must be universal and captured by models of solid-state creep (Mulyukova and Bercovici, 2020). Creep laws are deduced from rock deformation experiments, which provide measurements of stress-strain rate relationships (flow laws) and microstructure, and are corroborated by theories of motion of crystalline defects (vacancies, dislocations, grain boundaries, etc.). The defects continuously evolve, interact, and alter the rheological properties of deforming rocks. For example, changes in grain size and dislocation density change the relative contribution to strain from diffusion or dislocation creep. This can be represented on a deformation map constructed from experimentally determined flow laws, and whose axes can include grain size, dislocation density, and stress. One of the most obscure regions of the deformation map is the field boundary, where multiple deformation mechanisms make comparable contributions to strain and thus cannot be easily distinguished. I will present a new model where different creep mechanisms can co-exist and interact with each other, providing a microphysical basis for composite laws of diffusion and dislocation creep. In the new model, diffusion of vacancies is sensitive to stress-variations induced by grain boundaries and dislocations. Furthermore, the model distinguishes between the two main components of dislocation motion, namely dislocation glide and climb. While glide and climb velocities are commonly averaged and combined in Orowan-type models, they occur in different directions relative to the slip plane, and involve different micro-mechanisms (motion of kinks and jogs) with arguably different activation enthalpies and stress dependencies. I model dislocation climb as a diffusive creep mechanism, in which dislocations act as vacancy sources and sinks. For dislocation glide, I account for the fact that glide motion slows down with increasing dislocation density, as it gets impeded by the presence of differently oriented dislocations. Deformation map constructed from this new composite creep model differs from previous stress-strain rate relationships, for example in that it predicts effective stiffening as material transitions from diffusion to dislocation creep regimes (Figure 1). Finally, the new deforma- tion map is not restricted to steady state conditions, but readily captures transient microstructural changes (Mulyukova and Bercovici, 2022) and resultant changes in rheological properties (Mulyukova and Bercovici, 2018). Transient rheolog- ical properties are particularly relevant for modeling of relatively rapid geodynamic phenomena, such as deformation at tectonic plate boundaries through different stages of an earthquake cycle.



Figure 1: Steady state deformation map generated with (left) previously published creep parameters (Hirth and Kohlstedt, 2003; Kirby and Kronenberg, 1987), and (right) the new composite creep model. For this example, we assumed a temperature of 1200 K. On the left plot, the straight black line marks the field boundary, at which strain rates accommodated by grain boundary diffusion and dislocation creep (averaged glide and climb) are equal. On the right plot, blue line marks the field boundary where strain rate by grain boundary diffusion is equal to that by dislocation climb, while the red line marks the field boundary where strain rate by grain boundary diffusion is equal to that by dislocation glide.

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#### **\*** Invited speaker

## A coupled model for phase mixing, grain damage and shear localization in the lithosphere: Comparison to lab experiments

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The occurrence of plate tectonics on Earth is rooted in the physics of lithospheric ductile weakening and shear-localization. The pervasiveness of mylonites at lithospheric shear zones is a key piece of evidence that localization cor- relates with reduction in mineral grain-size. Most lithospheric mylonites are polymineralic and the interaction between mineral phases, such as olivine and pyroxene, especially through Zener pinning, impedes normal grain growth while possibly enhancing grain-damage, both of which facilitate grain-size reduction and weakening, as evident in lab experiments and field observations. The efficacy of pinning, however, relies on the mineral phases being mixed and dispersed at the grain scale, where well-mixed states lead to greater mylonitization. To model grain mixing between different phases at the continuum scale, we previously developed a theory treating grain-scale processes as diffusion between phases, but driven by imposed compressive stresses acting on the boundary between phases. Here we present a new model for shearing rock that combines our theory for diffusive grain mixing, two-dimensional non-Newtonian flow and two-phase grain damage. The model geometry is designed specifically for comparison to torsional shear-deformation experiments. Deformation is either forced by constant velocity or constant stress boundary conditions. As the layer is deformed, mixing zones between different mineralogical units undergo enhanced grain-size reduction and weakening, especially at high strains. For constant velocity boundary experiments, stress drops toward an initial piezometric plateau by a strain of around 4; this is also typical of monophase experiments for which this initial plateau is the final steady state stress. However, polyphase experiments can undergo a second large stress drop at strains of 10-20, and which is associated with enhanced grain mixing and resultant grain-size reduction and weakening. Model calculations for polyphase media with grain mixing and damage capture the experimental behavior when damage to the interface between phases is moderately slower or less efficient than damage to the grain boundaries; other factors such as distribution and bulk fraction of secondary phase, as well as grain-mixing diffusivity also influence the timing of the second stress drop. For constant stress boundary conditions, the strain-rate increases during weakening and localization. For a monophase medium, there is theoretically one increase in strain-rate to a piezometric steady state. But for the polyphase model, the strain-rate undergoes a second abrupt increase, the timing for which is again controlled by interface damage and grain mixing. The evolution of heterogeneity through mixing and deformation, and that of grain-size distributions also compare well to experimental observations. In total, the comparison of theory to deformation experiments provides a framework for guiding future experiments, scaling microstructural physics to geodynamic applications, and demonstrates the importance of grain mixing and damage for the formation of plate tectonic boundaries.

## Detachment fault growth modulated by brittle softening and ductile flow in (ultra)slow-spread oceanic lithosphere

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Mid-ocean ridges (MORs) display a variety of normal fault shapes and offsets, which have been primarily linked to variability in magma supply. However, because most modeling studies of MOR tectonics have relied on idealized representations of the oceanic lithosphere (e.g., an elastic-brittle layer overlying a weak asthenosphere), lithospheric strength profiles remain a poorly understood control on seafloor spreading modes.

We approach this question by focusing on two end-member styles of ultraslow and slow spreading: quasi-amagmatic sections of the South-West Indian ridge (SWIR), and partially-magmatic segments of the Mid-Atlantic Ridge (MAR). SWIR seafloor is shaped by large-offset detachment faults formed in a "flip-flop" pattern (Sauter et al. 2013), whereas the MAR displays multiple, axis-facing oceanic core complexes (Escartín et al., 2008). The two systems have contrasted strength profiles, with a colder thermal regime and a thicker ( $\approx$  15 km) seismogenic zone at the SWIR, and a weaker, melt-rich asthenosphere at the MAR.

We use 2-D numerical models (Olive et al., 2016) with self-consistent thermal evolution to investigate how the rheological layering of the lithosphere influences the growth of a detachment fault. Brittle deformation is modeled as Mohr-Coulomb plasticity with strain softening of friction and cohesion. Ductile deformation follows experimentally-determined flow laws, or is assigned a constant low-viscosity to represent a weak asthenosphere endmember. In this latter case, our simulations produce 3 faulting regimes: (1) long-lived detachments, (2) sequential horst formation, or (3) inefficient strain localization. We find that stable detachments are favored by a strong friction contrast between the fault zone and surrounding lithosphere. This is consistent with previous studies that employed a fixed thermal structure (Lavier et al., 2000), and interpreted this behavior as softening overcoming the delocalizing action of lithospheric flexure.

To further explore this idea, we consider strength profiles that include a viscous lower lithosphere of non-negligible strength. This yields similar faulting regimes, but impacts the conditions for regime transitions. Specifically, forming stable detachments requires a greater degree of softening, i.e., a greater friction and/or cohesion contrast between faults and bulk lithosphere. We use these results to quantify the contribution of the ductile lithosphere to strain defocusing, thereby extending standard models of MOR faulting to more complex yield strength profiles



Figure 1: Long detachment fault in a thick lithosphere

## **Coble Creep May Control Lower Mantle Rheology**

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Constraining the dynamics of Earth's silicate rich lower mantle informs our understanding of the entire planet. Of the lower mantle's set of phases, MgSiO3 bridgmanite is by far the most influential. Occupying up to 70% of the Earth's lower mantle volume, the ubiquity of this mineral suggests that it controls much of the lower mantle's thermal and chemical transport. Bridgmanite is stable at depths exceeding 660 km following the decomposition of ringwoodite to (Mg, Fe)SiO3 and (Mg, Fe)O. Currently, the dominant deformation mechanism of Earth's lower mantle has long been speculated. Until recently, the lack of seismic anisotropy throughout much of the lower mantle has led many to suggest that diffusion creep is preferable to dislocation creep, in which the latter typically leaves a seismically observable signature because of the crystal preferred orientation generated by specific crystallographic slip systems. Nevertheless, this stance has recently been questioned due to the possibility of dislocation climb, which, unlike dislocation glide, generates no seismic anisotropy. The distinct advantage of dislocation creep for geodynamic models is the lack of dependence on the grain size, a much-contested parameter. Furthermore, unlike diffusion creep, dislocation creep adheres to a linear dependence on the system's shear stress. This property facilitates the propensity for dislocation creep to generate low viscosities under conditions of high stress.

Nevertheless, both pure climb creep and Nabarro-Herring creep are intrinsically rate limited by the slowest diffusing species within the lattice. Thus, models suggest both Nabarro-Herring and pureclimb require relatively high vacancy concentrations,  $X_V$ , to explain the Earth's observed viscosity profile, greater than  $X_V = 105$ . The incorporation of hydrogen may generate the most likely sources of such vacancies. Another possible explanation is that materials could be deforming via Coble creep. This diffusion mechanism facilitates the propagation of vacancies and atoms along grain boundaries rather than through the lattice interior. However, to date, relatively poor constraints have been placed on the essential parameters of grain boundary diffusivity and width, not to mention the mean grain size of the lower mantle. Mineral physics has strengthened our rheological understanding of the lower mantle through computational and experimental approaches alike. Deformation experiments performed in either diamond anvil cell or D-DIA apparatus allow for the in-situ measurement of stress-strain relations. Such experiments performed on mantle minerals and analogues can be used in conjunction with microstructure analysis of quenched samples.

On the other hand, computational methods have modelled the kinetics of processes such as diffusion and dislocations, and more recently, grain boundaries. Such approaches have led to an enhanced understanding of the different pathways through which atoms migrate, as well as the relative strength of slip systems within lower mantle minerals. Grain boundaries have shown to influence the rheology of polycrystalline aggregates through the nucleation of dislocations and the migration of interfaces. Nevertheless, it is through the process of Coble creep that the role of grain boundaries in Earth materials is most important. Coble like its lattice counterpart, Nabarro-Herring, deforms a material through the diffusional flux of atoms and vacancies between different surfaces. However, unlike Nabarro-Herring, Coble creep is an order of magnitude more sensitive to the grain size of the medium. Furthermore, grain boundaries typically facilitate faster diffusion along the interface when compared to the lattice interior, a process that further controls wider properties such as ionic conductivity.

This work utilises a developed Machine Learning Potential to establish low energy grain boundary
structures for MgSiO3 bridgmanite at six different orientations. Following the analysis of grain boundary properties such as width, energy and structure, the diffusivity of the grain boundary region is obtained through large scale molecular dynamics calculations and the mean squared displacement analysis. The properties of grain boundary width and diffusivity are then used to place constraints on the grain-size dependent viscosity of the lower mantle via the Coble Creep formula.

## Analysis of strain-dependent weakening and hardening processes with applications to cross-scale geodynamic problems

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The formation and maintenance of narrow, lithospheric shear zones and their role in plate tectonics remain one of the major problems in geodynamics. Strain-localization is affected by weakening and hardening processes in the ductile and brittle regime. However, the causes and consequences of localization and weakening remain debated, even though tectonic inheritance and strain localization appear to be critical features for plate boundary evolution.

Here, we analyze the efficiency of strain localization for a strain-dependent weakening and hardening (SDWH) rheology in thermo-mechanical experiments with kinematic boundary conditions using different types of strain weakening (plastic- and viscous-strain softening). Such a parameterized rheologies successfully mimic more complex transient weakening and hardening processes, akin to a grain-size-sensitive composite (diffusion and dislocation creep) rheology. In addition, the SDWH rheology allows for memory of deformation. This enables self-consistent formation and reactivation of inherited weak zones within the lithosphere and sustains those weak zones over an extended period.

We further analyze the resulting shear zone patterns on small spatial scales and seek to answer the questions: What is the typical, effective intensity of strain localization? What are the dimensions of the resulting shear zones? Are such shear zones mesh-dependent in numerical models and, if so, can we exploit existing regularization approaches for the SDWH rheology?

We also use such SDWH rheologies for global mantle convection computations and analyze how such a SDW rheology affects the surface dynamics and the time-dependence of plate reorganization and heat transport in 3-D spherical, visco-plastic, thermo-mechanical models using the well-benchmarked community code CitcomS. Reactivation within the models occurs in two different ways: a), as a guide for laterally propagating convergent and divergent plate boundaries, and b), formation of a new subduction zone by reactivation of weak zones. A longer rheological memory results in a decrease in the dominant period of plate reorganizations due to less frequently formed new plate boundaries. These results show the importance of a rheological memory for the reorganization of plates, potentially even for the Wilson cycle.

# Characterization of deformation localization & quantification of feedbacks arising from non-newtonian mantle viscosity

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Deformation localization into initially undeformed, strong plate interiors is a key process to form new plate boundaries. Such a localization process occurs through a weakening that can arise from various mechanisms: tectonic inheritance and strain localization (e.g. reduced grain size, anisotropic structures), viscosity reduction when a given (yield) stress is overcome, shear heating, etc. Here, we explore an alternative, but potentially complementary process: deformation localization associated to a non-newtonian viscosity (dislocation creep) in the cold lithospheric mantle.

Solomatov (1995) proposed that stagnant-lide convection was the dominant mode for a nonnewtonian viscosity ; however we propose here to test to localization potentiel of a new lowtemperature dislocation creep parameterization - yielding lower viscosities than the classical high-temperature power-law (Gouriet+ 2019 ; Garel+ 2020). Indeed, positive feedbacks between deformation, viscosity, velocity and temperature are very sensitive to the rheological parameterisation governing deformation partitioning between newtonian and non-newtonian viscosities.

We analyze, in simple dynamical set-ups (e.g. sphere sinking or rising, simple shear) with variable rheological parameterization, the resulting deformation pattern, and quantify both a localization length scale and a (local) weakening factor. We also analyze, in a subduction simulation featuring a stretched upper plate, the chronology between thermal upwelling and deformation localization.

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# Narrow, fast, and "cool" mantle plumes caused by strain-weakening rheology in Earth's lower mantle

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The rheological properties of Earth's lower mantle materials are key for mantle dynamics and planetary evolution. The main rock-forming minerals in the lower mantle are bridgmanite (Br) and smaller amounts of ferropericlase (Fp). Bridgmanite minerals are intrinsically much stronger than ferropericlase minerals, resulting in significant variations in lower-mantle rheological behaviour depending on the quantity and degree of interconnectivity of the weak phase. The resulting effective bulk rock viscosity decreases with accumulating strain when the weaker Fp minerals become elongated and eventually interconnected. This implies that strain localisation may occur in Earth's lower mantle, which would in turn influence the pattern of mantle flow and could potentially aid the preservation of compositionally distinct, "hidden" reservoirs. So far, there have been no studies on global-scale mantle convection in the presence of such strain-weakening (SW) rheology.

Here, we present high-resolution 2D numerical models of thermo-chemical convection in spherical annulus geometry including a new strain-weakening (SW) rheology formulation for lower-mantle materials. This macro-scale SW rheology is based on micro-scale rheological behaviour found in prior studies, and combining rheological weakening and healing terms. We determine the effects of SW rheology on the planform of mantle flow, the mixing of chemical reservoirs, and the dynamics of mantle plumes.

We find that, in particular, plume conduits are weakened and act as lubrication channels which allow for the rapid ascent of mantle material. Their thermal anomalies and geometries are significantly different than those of mantle plumes which are not rheologically weakened. Moreover, larger thermochemical piles at the base of the mantle are stabilised by SW rheology, with implications for preservation of chemically-distinct materials over long timescales. Finally, we put our results into context with existing hypotheses on the style of mantle convection and mixing. Most importantly, we suggest that the new kind of plume dynamics may explain the discrepancy between expected and observed thermal anomalies of deep-seated mantle plumes on Earth.



Figure 1: (a) Variation of the bulk viscosity of Br-Fp mixtures as a function of Fp fraction for two end-member textures "load-bearing framework" (LBF) and non-linear "interconnected weak layers" (IWL). Adapted from Ballmer et al. (2017, *Nature Geosciences*, DOI: 10.1038/NGEO2898).
(b) Suggested mantle convection dynamics in which shear localisation of weak Fp grains induces weak layers of "interconnected frameworks" (IWL) along slabs and plumes, and mixing is less efficient for the bridgmanitic "load-bearing framework" (LBF) part of the lower mantle, potentially promoting the preservation of long-lived geochemical reservoirs. From Chen (2016, *Science*, DOI: 10.1126/science.aad7813).

### Using composite rheology models to explore the interplay between continent formation, surface erosion, and the evolution of plate tectonics on Earth

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Following the magma ocean solidification stage, a variety of tectonic regimes have been proposed for the early Earth albeit without any consensus: heat-pipe tectonics, plutonic-squishy lid, stagnant lid. Furthermore, the rheological changes required to make the (supposedly gradual) transition to modern style plate tectonics on Earth remain hotly debated. Also, different estimates of mantle potential temperature for the Archean have been proposed.

Recently, it has been proposed that sediments accumulated at continental margins as a result of surface erosion processes could have acted as a lubricant to stabilise subduction and aid with the initiation of plate tectonics after the emergence of continents around 3 Ga (Sobolev and Brown, 2019). It was further suggested that subduction zones were already present at that time but were likely initiated only above hot mantle plumes. This tectonic regime of regional plume-induced retreating subduction zones was very different from the modern type of plate tectonics, but nevertheless might have been efficient in production of early continental crust and recycling of water and pre-existing crust into the deep mantle.

In this work, we test this hypothesis of surface-erosion controlled plate tectonics preceded by plume-induced retreating subduction tectonic regime in global compressible convection models with composite rheology (diffusion creep and dislocation creep proxy). We decrease the effective frictional strength of the oceanic lithosphere to mimic the lubricating effect of sediments in the late Archean and after the Neoproterozoic glaciation. These models self-consistently generate oceanic and continental crust while considering both intrusive (plutonic) and eruptive (volcanic) magmatism (Jain et al., 2019). We also investigate the influence of lower mantle potential temperatures during the Archean on crust production and compare our results with geological data.

When compared to models with just diffusion creep, the models with composite rheology result in more efficient mantle cooling, higher production of continental crust, and higher recycling of basaltic-eclogitic crust through subduction, delamination, and dripping processes. These models are able to reproduce the cooling history of the Earth and also show higher mobilities (Tackley, 2000), which have been previously shown for diffusion creep models only with low surface yield stress values (Lourenço et al., 2020). Models initialised with lower mantle potential temperatures show an effect on the initial growth of TTG rocks over time. However, no considerable differences in terms of total crust production or mantle cooling are observed.

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# Incorporating olivine CPO-related anisotropic viscosity into 3D geodynamics simulations

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Olivine, the main rock-forming mineral of Earth's mantle, responds to tectonic stress by deforming viscously over millions of years. During viscous creep, olivine grains can rotate and deform, obtaining crystallographic preferred orientation (CPO). Because the intrinsic mechanical properties of olivine are anisotropic, areas in the mantle with strong olivine CPO will have anisotropic elastic and viscous properties. While CPO-related elastic anisotropy is well known and easy to observe by seismic waves, the geodynamic implications of upper-mantle viscous anisotropy remain enigmatic.

According to laboratory experiments on olivine, we expect that deformation occurs more easily when shear is parallel to, rather than across, the mean CPO (olivine a-axis direction). When strong CPO is present in the mantle, the differences in viscosities depending on the direction of deformation can be up to 2 orders of magnitude. However, the directional dependency of lithospheric and asthenospheric viscosity is rarely addressed in (3D) geodynamic models.

The open-source modeling package ASPECT has the possibility to handle viscosity as a tensor, and hence allows for modeling with anisotropic viscosity (AV). Previously, this feature has been used in a 2D setting, where AV was present due to shape preferred orientation created by dike intrusions (Perry-Houts and Karlstrom, 2019). However, a 2D method is not sufficient to model olivine related AV because the CPO of olivine tends to exhibit orthorhombic symmetry. Integrating anisotropic viscosity into 3D models would also allow us to use the actual laboratory-based parametrizations of the olivine slip-system activities and texture parameters when incorporating the CPO evolution and AV into a geodynamic model.

Here, we present the process for implementing the micromechanical model of olivine AV (described by Hansen et al., 2016) into ASPECT and combining it with a CPO evolution model (D-REX by Kaminski et al., 2004; integrated into ASPECT by Fraters and Billen, 2021). Our goal is to create an open-access tool within ASPECT that allows CPO to develop and affect the asthenospheric or lithospheric mantle viscosity, which will improve modeling a wide range of geodynamic problems. First, we use a box model to test the AV calculations against the results from Király et al., (2020), where the same micromechanical model was used (in MATLAB) on a set of olivine grains assuming simple shear. Then, following the examples in Fraters and Billen (2021), we will test the addition of AV in a corner flow and a subduction setup, in which we can compare not just the stresses and effective viscosities, but also CPO and model evolution, against (isotropic) models without AV.

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# The effect of grain size reduction for the origin of the mid-lithosphere discontinuity

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In the last decades, the high heterogeneity of the lithospheric mantle in terms of its physical properties and chemical compositions has been widely documented by geophysical, petrological, and geochemical studies. A sharp discontinuity in seismic velocity (2-10% reduction over no more than 30-40 km) is detected at 60 - 160 km depth in the continental lithosphere and at an average depth of 70 km in the oceanic lithosphere. Several models have been proposed for the genesis of this mid-lithosphere discontinuity (MLD) that include (1) the presence of partial melts or fluids, (2) layered anisotropy, (3) layered composition, and (4) elastically accommodated grain boundary sliding. However, all of these models have some limitations and cannot explain all the characteristics of the MLD. Here we propose a new model for the genesis of the MLD and explore its mechanism through thermomechanical numerical modeling combined at subduction zones. In the model, the deforming lithospheric mantle is affected by grain size reduction and growth processes. Numerical results show that the lithospheric deformation induced by subduction causes the grain size to sharply decrease within the brittle/ductile transition zone over significant regions inside the lithosphere, which is a possible barrier zone to accumulate the upwelling volatiles (e.g.,  $H_2O$ and  $CO_2$ ). Furthermore, the enriched melts/volatiles at Lithosphere-Asthenosphere Boundary (LAB), induced by small-scale convection, slab bending, or slab dehydration, is a critical factor in providing the upwelling volatiles that causes the mid-lithosphere discontinuity. The depth of the accumulated volatiles zone depends mainly on the age of the oceanic lithosphere and the thickness of the continental lithosphere and is consistent with the observations.

## The Lattice Boltzmann Method to simulate mantle convection with plastic rheology and the emergence of plate tectonics

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The simulation of mantle convection and plate tectonics is a challenging task for traditional methods of numerical solution to PDE's[1] due to the need to model sharp and large viscosity contrasts and highly nonlinear plastic rheologies. We present a thermal Lattice Boltzmann Method (LBM)[2] based on simulating the movement and collision of mass and energy densities on a discrete lattice as an alternative to PDE-based solutions, and we demonstrate that the LBM is capable of modelling the emergence of plate tectonics.

In past work[3, 4, 5], we demonstrated that the thermal LBM is capable of modelling a wide range of Rayleigh numbers in the range of 1700  $\rightarrow$  10 10 and Prandtl numbers in the range 1  $\rightarrow$  10<sup>4</sup>, and is able to simulate strongly temperature dependent viscosity[5] which leads to pulsating plumes. In this work, we introduce a strongly nonlinear plastic rheology of form  $v_{plastic} \propto \dot{e}^{-N}$  where *epsilon* is the shear strain rate, and we demonstrate – as expected — that strongly plastic rheology can lead to the emergence of plate tectonics. Specifically, we initialized a 2D model of size 512 × 256 where the model was heated at the lower boundary and cooled on the upper boundary. The viscosity and thermal diffusivity were calculated for a Rayleigh number of  $Ra = 4 \times 10^6$  and a Prandtl number of  $Pr = 10^3$ , and the plasticity exponent was set to a small value of N = 1 (i.e. weakly plastic). We then initialized an upper layer about 20% of the depth of the model with a strong plasticity (N = 4) and a 50× lower viscosity  $\Rightarrow Pr = 20$ . We then performed a 10 6 time step simulation in which we initially observed a largely decoupled two-layer convection system followed by the emergence of plate tectonics. Namely, we found that there was plate-like motion at the upper surface, complete with plate spreading centres and subduction zones such as in Figure 1.

In conclusion, the thermal LBM's ability to model large and sharp viscosity contrasts and nonlinear rheologies such as plastic, potentially allows it to model the complete dynamics of the earth from a lava world through to the present solid earth with plate tectonics. The thermal LBM offers a valuable alternative to PDE based solutions for simulating mantle convection and plate tectonics, and it may help lead to improved understanding of the emergence of plate tectonics and the conditions required to develop tectonically active exoplanets.



Figure 1: Snapshot at time step 572,000 of the horizontal component of velocity (left) and the vertical component of velocity (right) showing the emergence of plate tectonics. Namely, thin plate-like movement in the top part of the upper layer with a subduction zone at x 100 and a spreading center at x 370.

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## Effect of heterogeneous grain-growth in Earth's mantle

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Grain size ( $\mathcal{R}$ ) is one of the key factors controlling the rheology and dynamics of the Earth's mantle [1, 2]. The mantle is composed of polycrystalline grains that often deform within the grain size sensitive creep regime, i.e., diffusion creep. Hence, a small change in the grain size can modify the viscosity ( $\eta$ ) to a significant extent, as  $\eta \propto \mathcal{R}^n$ , where *n* varies between 2 and 3. However, the effect of grain size-dependent rheology on the dynamics and evolution of the mantle is so far not studied extensively using mantle convection models. Some of the previous studies used grain size evolution data obtained for upper mantle materials (e.g., olivine) [3]. Thus, the dynamics using grain-growth data applicable to the lower mantle remained unconstrained. With more advanced experimental methods, we have now obtained the grain-growth kinetics data for bridgmanite co-existing with ferropericlase [4], which is equivalent to the lower mantle's composition.

We develop numerical models incorporating composite rheology and grain size kinetics in 2D spherical annulus geometry employing the finite volume code StagYY. For this purpose we impose two kinds of grain growth kinetics in the upper and lower mantle. We employ for the upper mantle (<660 km) grain-growth parameters for olivine [5] and for the lower mantle we use grain-growth parameters for bridgmanite/ferropericlase [4]. The combined parameters show faster grain-growth in the upper mantle and a slow grain-growth in the lower mantle. Our preliminary results covering 4.5 Gyrs of evolution suggest that grain size-dependent rheology can potentially stabilise large low shear wave velocity provinces in the lower mantle and provide a suitable viscosity that allows for a change of tectonic mode from squishy-plume lid to mobile lid regime (Fig. 1).



Figure 1: Snapshot of temperature, viscosity and grain size fields at 3.4 Gyrs from a model incorporating grain size-dependent rheology.

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### Micro-scale dependent, time- and space-evolving rheologies: key for ductile strain localization in geodynamical models

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Strain localization is the rule rather than the exception in the lithosphere. Yet, modelling strain localization in the ductile field, which represents on average 90% of the lithosphere, remains a real challenge. Analysis of observations of ductile strain localization at various spatial scales in nature and experiments shows that heterogeneity in the mechanical behaviour is key for strain localization. This heterogeneity exists at all scales, in particular at small ones, and evolves in response to the mechanical fields. In the ERC RhEoVOLUTION, we posit that poor representation of this heterogeneity and its evolution during deformation is the locking point for generating strain localization in geodynamical models. We propose therefore to examine how strain localization may arise in rocks deforming by ductile processes by associating a stochastic description of the mechanical properties of the medium with simple laws describing how these properties evolve in response to the resulting heterogeneous deformation (variations in stress and strain rate). The first results show that random variation in the rock mechanical properties (here, a strength variable describing a resistance to deform by dislocation creep) implemented in a stochastic manner in a FE model (random drawings from a truncated Gaussian distribution at fixed time intervals) produces, for simple boundary conditions and constant temperature, a strain rate field characterized by shear bands at 45° to the compression direction. The width of the shear bands is controlled by the size of the rheological heterogeneities. Their spacing results from the interactions between the perturbations in the strain field induced by the different heterogeneities; for a random distribution there are multiple wavelengths between 2-10 times the size of the heterogeneities. If the stochasticallydescribed material property varies as a function of the local work (or work rate), strain localization at scales larger than the initial characteristic length scale of the rheological heterogeneity field may develop. A few shear zones lengthen, coalesce, and sometimes widen, dominating the whole system. The evolution is controlled by the material properties (characteristics of the probability distribution function) and their evolution (imposed change in the PDF, frequency of the drawings, imposed temporal and spatial correlations). The present results, although preliminary, show that stochastic time-varying descriptions of the ductile rheology of rocks may generate spontaneous strain localization in numerical models. This approach is thus a powerful tool for investigating the role of different physico-chemical processes on strain localization.



Figure: Example of a simulation with a work-controlled evolution of the material strength PDF. Center: Strain rate field after 25% of bulk shortening along the X direction showing a marked strain localization (two orders of magnitude of variation in strain rates). Inserts at top and bottom left display the initial, which is characterized by a random variation of the Peierls stress of  $2\pm0.5$  GPa in a dislocation creep flow law for olivine with both a power and an exponential dependence on stress, Gouriet et al. EPSL 2019) and the final material strength fields. Insert at top right displays the shear (xz) component of the strain field at the end of the simulation. Average bulk strain rate  $2 \times 10^{14}$  s<sup>-1</sup>; constant temperature of 1000K.

### Olivine texture evolution under a simple deformation scheme: Comparing different numerical methods of LPO calculation

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The development of olivine texture, and in particular lattice preferred orientation (LPO), has been implemented in many numerical modeling tools to predict seismic anisotropy, which places constraints on mantle dynamics. However, a few recent studies have linked olivine texture development to its mechanical (viscous) anisotropy, which in turn can affect deformation rates and also the resulting texture. To study the effect of anisotropic viscosity (AV) and LPO evolution on geodynamic processes, it is important to know the role of AV and LPO and the differences between the numerical methods that calculate them.

We use and compare two methods of LPO-tracking: D-Rex [1] and the Modified Director Method (MDM) [2]. D-Rex is a polycrystal type model used to calculate texture evolution for olivine aggregates based on a kinematic approach. The MDM parameterizes the olivine LPO formation as relative rotation rates along the slip systems that participate in the rotation of olivine grains due to finite deformation. When MDM is coupled with a micromechanical model for olivine AV, it allows the anisotropic texture to modify the viscosity. We compare the olivine textures predicted by the MDM both with and without a coupled micromechanical model (MDM and MDM+AV) and textures predicted by D-Rex in two well-understood 3D models: a shear box model and a subduction model.

In general, we observe a decrease in the effective viscosity and a faster texture development using the MDM+AV method, while all three models run until the texture saturates and reaches a similar texture score. In the subduction model, the effective viscosity a particle experiences fluctuates throughout the model, and in models using D-Rex and MDM+AV, the same particle experiences a variety of different effective viscosities as it moves through the subduction zone. This suggests that adding anisotropic viscosity to subduction models may significantly modify the mantle flow pattern in the vicinity of subduction. The difference between models with and without AV suggests that it is important to include the effect of AV in modeling systems where mantle flow varies significantly in time and space, such as subduction zones.

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# Coupling thermodynamic and thermomechanical codes in Julia to study magmatic processes

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One of the continuing trends in geodynamics is to develop codes that are suitable to model magmatic processes with an increasing level of self-consistency. Developing such models is particularly challenging as most magmatic processes are multiphysics problems, and require coupling between thermal, porous, mechanical and chemical processes.

One of the first difficulties in modeling magmatic systems is obtaining thermodynamic properties, and most importantly phase assemblages. Thermodynamic data for realistic bulk compositions features a very high dimensionality. Therefore, interpolating thermodynamic properties from a pre-computed database is not efficient, while present Gibbs energy minimizers are not fast enough to calculate the local thermodynamic properties in real time and/or have a range of failed minimizations. Therefore, we developed a code, (Mineral Assemblage Gibbs free Energy Minimizer - MAGEMin). which computes the stable assemblage for given pressure, temperature and bulk-rock composition and is stable, fast and works on parallel machines.

Apart of obtaining the thermodynamic properties, much of the difficulty of solving magmatic problems in a fully coupled manner is, that a stable and computationally efficient solution scheme is hard to find. This is because of the strongly nonlinear feedbacks and the large numbers of independent variables, that such formulations require. Therefore, many previous models include simplifying assumptions to reduce nonlinearities or to replace two-way by one-way couplings. In this talk, we present two different methods to self-consistently include latent heat and volume change effects of partial melting or phase transitions. One method is based on the use of effective thermodynamic properties and is well suited to model chemical systems with gradual changes in the phase assemblage (in the P-T space). The other method is based on the use of specific entropy and density as primary thermodynamic variables, which is suitable for sharp changes in the phase assemblage (in the P-T space).

We will discuss rarely quantified effects of the full thermodynamic coupling on an example of thermomechanical cooling of magma chambers in a compressible visco-elasto-plastic host, including thermal expansion, latent heat and volume change of crystallization.

All the codes presented here are written within a modular Julia framework, developed within the MAGMA ERC project, that permits easy future integration of the currently stand-alone software.

# Using graphics cards to solve forward and inverse problems in geodynamics

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Continuum mechanics-based modelling of large-scale problems in geodynamics requires huge computational resources to accurately capture spatial and temporal evolution over long time scales. Examples of such problems range from mantle convection, partial melt segregation, fluid transport and heat transfer, to seismic waves propagation. Over the last decades, the massive increase in processing capabilities of modern hardware such as graphical processing units (GPUs) made it possible to solve forward but also inverse problems at unprecedented resolution and in 3D.

In this workshop, we present concise and relatively easy to implement numerical techniques to solve coupled multi-physics problems using one to thousands of either Nvidia (CUDA) or AMD (ROCm) GPUs. We use the Julia language, which allows writing high-level code that executes with near-optimal performance comparable to hand-tuned C or Fortran code.

We explain the basics of the pseudo-transient (PT) method, which is a matrix-free iterative method. The PT method is easy to code, executes optimally on GPUs, and the resulting codes look close to mathematical notation. We will demonstrate the applications of the method to resolve important processes that serve as building blocks in geodynamical simulations, such as advection-reaction-diffusion and incompressible viscous and visco-elastic Stokes flow. We will explain how to achieve linear scaling of the solver by utilising over-relaxation and discuss the optimal choice of numerical parameters.

We will then demonstrate that the pseudo-transient method implementation is amendable to perform inverse modelling using the adjoint method. Thanks to the powerful code-generation capabilities of the Julia language, the necessary building blocks for the inverse solve can be generated automatically by leveraging automatic differentiation (AD). We will showcase a simple forward problem and then modify it to retrieve the spatial distribution of the property of interest, e.g., viscosity, that minimises the deviation of the model predictions from observations. We plan to make the workshop material freely accessible on GitHub (https://github.com/PTsolvers) to allow for self-guided experimentation.

### Breaking the lithosphere: how to combine shear and tensile plasticity with non-linear rheologies

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One of the great challenges involved in modelling the lithosphere is its plastic behavior, especially when dealing with compressible materials. Shear fractures are designated as mode 2 and 3 and can be described using a linear Mohr Coulomb envelope or a simplification of it like Drucker-Prager. Meanwhile, mode 1 fractures are created when the normal stresses become tensile and require another yield function, such as the Griffith criterion or a tension cap function.

While the governing equations are well known and widely employed in engineering codes, they are usually implemented in conjunction with linear rheologies, either elastic or linearly elastoviscous. Geodynamic systems, on the other hand, evolve on timescales where dislocation creep and other non-linear mechanisms are relevant. A numerically robust method that takes all those rheologies into account in a staggered finite difference discretization remains then a necessity. Here we present a composite yield function implemented with pressure-velocity formulation, capable of producing shear and tensile failure, fully coupled with a non-linear elasto-viscous rheology.

We have implemented this in a new code that employs PETSc through the recently updated PETSc.jl Julia interface, while utilizing the automatic differentiation tools available in Julia. We found this workflow to significantly reduce the development time of complex nonlinear coupled codes.

We will describe the implementation, propose regularization schemes and discuss benchmark cases and simple applications. We demonstrate Newton convergence for most cases.

## Lithosphere dynamics with frictional plasticity: Regularisations

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Frictional plastic rheology can explain the development, the architecture and the reactivation of fault systems. It is hence an important ingredient of geodynamic simulations that seek to predict the generation and evolution of high strain zones and plate boundaries. However the inclusion of frictional plastic rheology in geodynamic simulators is troublesome. For example, the satisfaction force balance becomes difficult, if not impossible, and numerical solutions may depend on grid resolution. In order to alleviate these issues, regularisation techniques were designed in the engineering community. We have tested three commonly employed regularisation approaches: viscoplasticity, gradient plasticity and Cosserat-type regularisation. These three approaches were implemented in a single numerical code based on an accelerated pseudo-transient solving strategy. Thanks to this solving strategy, we were able to explore the effects of different regularisations within the same context. We have simulated shear banding on the kilometer scale using different initial configurations. The considered methods all successfully resolve shear banding, satisfaction of force balance and convergence upon grid refinement. The simplest regularisation approach to implement in geodynamic codes is viscoplastic regularisation. However more reliable stressstrain measurements and shear band patterns are obtained with, yet, more expensive gradient and Cosserat-type regularisation. We discuss the relative benefits and their potential combinations for the purpose of gedynamic modelling.



Comparison of shear banding patterns computed with the different regularisation approaches and for different numerical resolutions. Low resolution (LR, 94 × 62 cells (A to C). Medium resolution (MR, 190 × 126 cells (D to F). High resolution (HR, 382 × 254 cells (G to I). The color map corresponds the value of accumulated strain. The same random cohesion field was used as initial condition.

## A higher-order accurate particle infrastructure for the community: Benchmarks and applications in geodynamics and engineering

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The reliability and predictive power of numerical models of the Earth's mantle and other planets rely on an accurate representation of the continuous rock properties in a discretized model. Due to their inherent suitability for modeling advection dominated processes, particle methods have been applied to track quantities such as the composition of solid rock and melt in the Earth's mantle, fluids in lithospheric- and crustal-scale models, light elements in the liquid core, and pollution in fluvial systems at the Earth's surface. Traditionally, particle algorithms often rely on a regular, structured background mesh, and are re-implemented and optimized for each individual software application.

Over the past years, we have developed a flexible, scalable, and efficient particle architecture that is open-source, application agnostic, and performs well in modern high-performance computing environments. In particular, it supports advanced computational methods such as an adaptively refined, unstructured, and dynamically changing background mesh, parallelization exceeding tens of thousand of compute cores, assigning arbitrary particle properties, and nonlinear solver schemes. This architecture is integrated into the free software library deal.II and has been used in traditional applications in the geosciences, as well as other fields, such as ion transport and mixing of granular flows.

We present three recent advances in our particle infrastructure. First, we have created two new dynamic benchmarks for transient Stokes flow with an analytical solution that allows us to quantify the accuracy of any advection method. We use these benchmarks to measure the accuracy of our particle algorithm as implemented in the ASPECT geodynamic modeling software. Second, we have developed a new slope-limited interpolation algorithm from particles to the numerical grid that reaches optimal accuracy at constant particle numbers while suppressing oscillations for discontinuous properties. Third, we illustrate the integration of our particle infrastructure into the open-source code Lethe-DEM, a discrete element software for modeling granular flows in chemical or geotechnical engineering. We provide the community with an accurate, scalable and efficient particle infrastructure as a tool to reliably model more complex geodynamic processes, such as elastic stresses, anisotropic fabric, melt composition, and material damage.



Left: Influence of different particle advection schemes on the evolution of small-scale convection (SSC) and grain size (background colors) underneath an oceanic plate. SSC develops earlier with less accurate advection schemes, illustrating the need for accurate particle methods. Right: Application of our particle methods in the discrete-element software Lethe-DEM, modeling the filling of a silo with granular material. Background colors show efficient parallel partitioning.

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## Free surface methods applied to global scale numerical geodynamic models

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The study of coupled Earth systems, and in particular the coupled interactions between the lithosphere, atmosphere, and biosphere, have received greater attention in recent years (Gerya et al. 2020). Interactions between these systems occur primarily at the surface, and are driven on the large scale by topographic and bathymetric evolution controlled by deep mantle processes. However, due to the large difference in length scales between the mantle and the surface, it is difficult to capture topographic evolution to a high degree of accuracy in existing global mantle convection models including a free surface boundary condition.

Global mantle convection models incorporating a free surface often employ a marker-in-cell technique with a layer of "sticky air" (i.e. material with the density of the air and sufficiently low viscosity, which is still much higher than that of real air) to characterise the surface. However, accurate topographic evolution using this method requires a high density of markers near the surface. This need for additional computational resources motivates alternative methods of tracking the interface between the air and rock layers, as is done frequently in existing multiphase fluid flow codes. Such interface tracking methods include the use of a Lagrangian surface marker chain with an appropriate remeshing procedure (van Keken, 1997), the use of a level-set function defined by the distance to the surface (Hieber & Koumoutsakos, 2005), or the introduction of a volume of fluid method with piecewise-linear interface reconstruction and a geometric advection routine (Katopodes, 2019).

We demonstrate toy models and benchmarks of these methods implemented in the Julia programming language within a framework suitable for inclusion within existing geodynamic models. Future work will involve the implementation of these methods within the existing code StagYY (Tackley, 2008) and benchmarking of results. Models of global scale topography and evolution produced using StagYY may then be used as a tool for further studies on the coupling of mantle dynamics with modelling of the landscape, and the evolution of the atmosphere and biosphere.

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### **Computational Infrastructure for Geodynamics – the next 5 years**

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Scientific computation is an integral part of solid Earth geosciences, especially in geodynamics and seismology, with computational models providing an essential link between observations and and a quantitative explanation of the Earth's interior and evolution. The Computational Infrastructure for Geodynamics was established in 2005 as a partnership between computational and solid-Earth science to advance computational modelling in geodynamics. In the past 17 years, we have developed and disseminated widely used, open-source codes for research and education in computational seismology, mantle convection, magma dynamics, short- and long-term lithospheric deformation, and geodynamo modeling. We have advanced the field by developing and disseminating scientific software based on best practices adapted from computational science and software engineering. Some examples of software and communities of users and developer supported include: PyLith to study short-term crustal deformation, ASPECT to study the Earth's mantle and lithosphere, Rayleigh to study stellar and planetary dynamics, and SPECFEM to simulate global and regional wave propagation.

We propose to continue to build upon this foundation in the next 5 years receiving guidance from our community in supporting the infrastructure for the development of sustainable software and software communities in enabling frontier research. Our efforts will focus on 4 cornerstones:

- 1. Modeling software: Providing powerful software to solve computational models, motivated by important science questions, and built on best practices in open-source software and scientific computing;
- 2. Computational workflows: supporting workflows that facilitate the set-up, execution, analysis, and exchange of complex computational models;
- 3. Training: Enabling a well-educated, well-trained, and diverse 21st century workforce that can effectively use and extend computational models for reproducible discovery and reuse, and that can fully exploit high-performance computing resources; and
- 4. Community: Building and sustaining a diverse and sustainable community of disciplinary and interdisciplinary researchers working together on challenging geoscience and software problems.

In support of these efforts, we host landing pages for open-source software projects that meet our best practices providing a resource for discovery of high-quality software; expert guidance for your software and community; and support for outreach including hackathons, tutorials, and notebooks. In addressing future challenges, we seek feedback on how our infrastructure and expertise can expand and partner with the community to meet future and current needs. Find us at: geodynamics.org



# Tools to build modular geodynamics codes in julia to simulate lithospheric and magmatic systems

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Julia is a relatively new scientific computing language that greatly simplifies writing new, fast, parallel codes on both CPU's and GPU's and is thus of considerable interest to the computational geodynamics community. It comes with a range of useful tools, such as automatic differentiation packages (e.g., Enzyme.jl or ForwardDiff.jl), which allow to automatically compute Jacobians to perform nonlinear simulations (in implicit code), or that can be used for uncertainty quantification or as part of an inversion algorithm (to fit models to data).

Here we will discuss our efforts in making Julia a development platform for geodynamic applications and for building models of the magmatic system, that significantly simplifies the process of going from a working solver to a production code. We are working on a range of packages that simplify certain steps that many geodynamics codes have in common:

- GeoParams.jl performs non-dimensionalisation and allows performing point-wise calculations for constitutive relationships (e.g., viscoelastoplastic rheologies, specifying density, melt parameterisations) which can be used along with other implicit/explicit solvers and different discretization techniques (FEM, staggered finite difference).
- GeophysicalModelGenerator.jl allows you to quickly collect geophysical/geological data of a certain region and create a model setup from that with a few simple steps.
- MAGEMin\_C.jl is a Julia interface to our new parallel thermodynamics code, MAGEMin, which is ideally suited to model the chemical evolution of magmatic arc systems, and more robust (and usually faster) than other widely used tools.
- PETSc.jl is the main interface from Julia to PETSc, which allows writing your code in Julia (while using automatic differentiation) while running it using the wide spectra of PETSc solvers (and run it in parallel). It will automatically install
- ParallelStencil.jl and ImplicitGlobalGrid.jl are packages that are devoted to solving stencils in a very efficient manner on (parallel) GPU or CPU machines, which scales to very large GPU-based high-performance computers. It is particularly efficient in combination with pseudo-transient iterative solvers.
- JustPIC.jl is our ongoing effort to add Particle-in-Cell advection schemes for GPU's and CPU's, which seamlessly integrates with ParallelStencil and ImplicitGlobalGrid.
- MagmaThermoKinematics.jl simulates the thermal evolution of magmatic systems following the intrusion of dikes/sills. It integrates with GeoParams.jl, which thus allows you to modify material parameters (constant density, density from phase diagrams, etc.) on the fly, with no need to change the code itself.
- LaMEM\_jll is a binary builder version of LaMEM that comes along with a parallel LaMEM version (and MPI+PETSc). It can directly be installed through the Julia package manager and downloads a binary version of LaMEM that works on all main operating systems and

can either be used directly from Julia or called from the command-line. There is thus no need for the (often painful) step of installing PETSc on your machine, which greatly lowers the barrier to use LaMEM in teaching or research.

## Multiple applications of MDoodz: 2-D Finite Difference/Markerin-Cell code

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The practical purpose of MDoodz 7.0 is to configure models and perform numerical simulations of geodynamic, tectonic and metamorphic processes at different spatial and temporal scales. This includes the simulation of the deformation of tectonic plates (collision and subduction zones, rifting, interactions with surface and mantle processes) as well as small-scale modelling of deformation of mineral phases.

MDoodz7.0 is a thermo-mechanical code based on the Finite Difference/Marker-in-Cell method. Non-linearities arising from visco-elasto-(visco)plasticity are treated by Newton iterations at both local and global levels (Duretz et al., 2021). The numerical solver for the mechanical processes can handle both incompressible and compressible flow (elasto-plasticity, phase transformations). Most recent developments include transient anisotropy based on the director vector approach (e.g. Mühlhaus, 2002) and interaction between phase transformations and plasticity (Yamato et al., 2022).

Here we present some selected tests and geodynamic modelling templates used in MDoodz7.0. Mechanical 'ShearTemplate' consists of a host/inclusion system in which deformation is induced by far-field pure shear and/or simple shear. The 'TopoBenchCase1' model shows the ability to simulate the evolution of free surface based on an analytical model (Crameri et al. 2012). 'ShearHeatingDuretz14' is a thermo-mechanical model of strain localisation induced by thermal softening. 'RiftingChenin19' is a basic model template used to simulate continental rifting.

One specificity of MDoodz7.0 is the ability to model anisotropic materials. Thus we show some simple simulations involving anisotropic flow and we discuss the potential role of anisotropy for large-scale geodynamic processes.



Fig. Example results of MDoodz mechanical and thermo-mechanical models. Left-top: Rifting Pauline ( $\epsilon_{ii}$  map), Right-top: ShearHeatingDuretz14 ( $\epsilon_{ii}$  map), Bottom-left and right: ShearTemplate (pressure map with velocity field directions) with simple and pure shear.

## Using Julia for the next generation of multi-XPU geodynamic codes

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Following the long-standing paradigm in HPC, computational geodynamic codes have been written in high-level statically typed and compiled languages, namely C/C++ and Fortran. The low productivity rates of these languages had led to the so-called "two-language problem", where many developers make use of dynamic languages such as Python or MATLAB to prototype their algorithms, before translating them into C/C++/Fortran. The Julia programming language aims at bridging the productivity and advantages of such dynamic languages without sacrificing the performance provided by static languages.

We propose the open-source and Julia-written package JustRelax.jl as a way forward for the next generation of geodynamic codes. JustRelax.jl is a production-ready API for the Stokes and thermal diffusion equations based on the embarrassingly parallel pseudo-transient method. Leveraging the high-performance and code-generation capabilities of Julia, JustRelax.jl relies on ParallelStencil.jl (https://github.com/omlins/ParallelStencil.jl) to provide an interface which is near-agnostic to the back-end system (CPU/GPU) that runs seamlessly in local shared-memory workstations and in distributed memory and multi-GPU HPC systems with minimal effort for the front-end user thanks to ImplicitGlobalGrid.jl (https://github.com/eth-cscs/ImplicitGlobalGrid.jl). Exploiting the code composability offfered by Julia, other key features for geodynamic codes are provided by other external open-source packages:

- GeoParams.jl (https://github.com/JuliaGeodynamics/GeoParams.jl): a package that provides a reproducible, lightweight, and optimized computation of different material properties (e.g. rheology, density, seismic velocity, etc.), handles automatic (non-)dimensionalization of the material parameters. This package supports both CPU and GPU devices and is entirely compatible with ParallelStencil.jl.

- JustPIC.jl (experimental): a package for the Particles-in-Cell method to track material properties. This package is carefully designed to provide an optimized and scalable advection scheme for staggered grids, employing ParallelStencil.jl to switch back-ends and ImplicitGlobalGrid.jl for distributed memory parallelism.

We finally present a collection of benchmarks that demonstrate the accuracy of the pseudotransient method to solve the Stokes equations for problems relevant to geodynamics, as well as scaling tests on both CPU(s) and GPU(s) back-ends.

## Towards building high resolution paleo elevation and climate maps for biogeodynamic modeling

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Driven through plate tectonics the continental and ocean basin configuration is changing constantly. This transformation is inherently linked to Earth's evolution of life, climate and landscape by erosion and through dispersal systems deposition. To study the effects and feedback between different systems throughout deep time detailed maps of topogra- phy, bathymetry and climate are necessary. Current elevation maps over the last 500 Ma have spatial resolutions in the order of 0.1° and an even lower resolution for climate data both with temporal resolutions of 10 Ma or lower.

To improve this and better investigate the evolution of life, biodiversity and systems like the CO 2 cycle we build upon the paleo DEMS [1] which provide digital elevation maps in 10 Ma steps with a 0.1° spatial resolution. Downscaling these maps and running fast fully coupled, mixed-resolution, general circulation model designed for high- throughput (FOAM, [2]) we obtain coarse (R15) climate data in 5 Ma steps for multiple CO 2 concentrations ranging between 100 and 3000 ppm for each continental configuration.

By using the CHELSA algorithm [3] we can statistically scale the most important climate variables, namely air surface temperature and precipitation back to the paleo DEMS resolution.

With this approach we can obtain comparatively high resolution climatic variables within a short amount of compu- tational time compared to general circulation models using a similar resolutions.

To finally capture the effect of precipitation and tectonic movement we run the gospl model [4] to investigate physical denudation by the influence of erosion and deposition of sediments. In this model we can use the jigsaw algorithm to create a mesh with a higher resolution, e.g. 100 km in the deep ocean ( $\leq$  -1000 m), 30 km across shelf margins ( $\leq$  -1000 m and <0 m), 15 km spacing for the continental domain and fit the digital elevation maps together with in GPlates computed velocity fields of tectonic plates as well as precipitation to this mesh.

This allows us to generate high resolution topographic maps over long time spans with a more realistic evolution of Earth's surface while forcing it to respect the original paleomaps given every 10 Ma and exploring the results for vastly different climates and at intermediary times in the order of 100 ka.

With this high spatial-temporal resolution approach combined with biogeographical models, we aim at understanding effects of major continental collision and breakup events in the global Wilson cycle for the evolution of both regional and global bio-diversity.

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### On the choice of finite element for applications in geodynamics

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Geodynamical simulations over the past decades have widely been built on quadrilateral and hexahedral finite elements. For the discretization of the key Stokes equation describing slow, viscous flow, most codes use either the unstable  $Q_1 \times P_0$  element, a stabilized version of the equal-order  $Q_1 \times Q_1$  element, or more recently the stable Taylor-Hood element with continuous ( $Q_2 \times Q_1$ ) or discontinuous ( $Q_2 \times P_{-1}$ ) pressure.

Conversely a handful of other numerical codes rely on triangular/tetrahedral elements, using the  $P_2 \times P_1$ , Crouzeix-Raviart ( $P_2^+ \times P_{-1}$ ) or MINI ( $P_1^+ \times P_1$ ) elements. However, it is not clear which of these choices is actually the best at accurately simulating "typical" geodynamic situations, especially buoyancy-driven flow.

Our recent publication (Thieulot & Bangerth, Solid Earth 13, 2022) provided a systematic comparison of all of the quadrilateral elements for the first time. We here repeat the exercise with triangular elements which we compare among themselves and against quadrilateral elements too. We use a series of benchmarks that illuminate different aspects of the features we consider typical of mantle convection and geodynamical simulations.

## TC1D: A new 1D thermal and thermochronometer age prediction model for quantifying rates of geodynamic and geomorphic processes

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Thermochronology is a dating method based on measuring ages that (typically) reflect the time since a mineral cooled below a system-specific temperature known as its effective closure temperature. The closure temperatures for many mineral thermochronometer systems (50-400°C) occur within the upper to middle crust, making this method suitable for quantifying rates of rock exhumation related to crustal tectonic and erosional processes. However, to calculate exhumation rates and how they relate to tectonic or erosional processes, an estimate of the depth to an effective closure temperature is needed. This depth can vary considerably due to many factors (e.g., advection of heat during exhumation, rock thermophysical properties, groundwater circulation, topography, etc.), and thus the depth estimation often requires some kind of model. Examples of popular models for interpreting thermochronometer data include (1) the thermal history model HeFTy (Ketcham, 2005), which calculates possible thermal histories that could produce a given age or set of ages, but does not allow for calculation of exhumation rates, and (2) Pecube (Braun, 2003), which is a sophisticated 3D thermokinematic numerical model, but requires users to compile the software, use a command-line interface, and can thus be challenging for new users.

Here we present TC1D, a new one-dimensional thermal and thermochronometer age prediction model that can simulate the effects of various geodynamic and geomorphic processes on thermochronometer ages. For example, TC1D can be used to explore how thermochronometer ages are affected by varying rock thermal properties, exhumation histories, thermal processes such as mantle delamination, or thermochronometer mineral properties. TC1D is written in Python and aims to be a tool that is easy to use like HeFTy but with direct estimates of exhumation rates from ages, while being less complex, faster, and easier for new users than Pecube. The thermal model uses either an implicit or explicit conservative finite-difference solution to the heat conduction equation including advection and heat production. The thermal history recorded during exhumation can be used to compute apatite and zircon (U-Th)/He and apatite fission-track ages, and goodness-of-fit values can be calculated based on a comparison to measured ages. TC1D also includes a batch mode that can be used to run many models to explore permutations of input parameter ranges. In the associated poster we provide an overview of the design of TC1D, some examples geological scenarios and their predicted thermal histories and thermochronometer ages, and the plans for future development of the software.

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Thermal and erosion histories, and predicted thermochronometer ages for a scenario with 2 km of exhumation in the first 45 Myr and 8 km of exhumation in the final 5 Myr of a calculation with TC1D.