LaMEM short course

17-21 02 2025 Heidelberg

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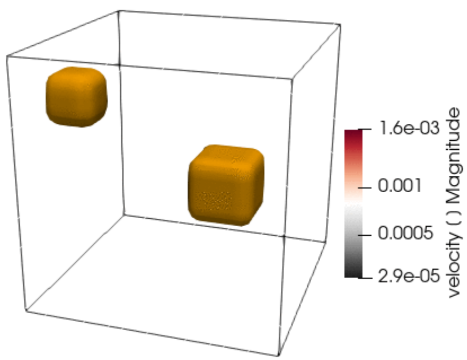
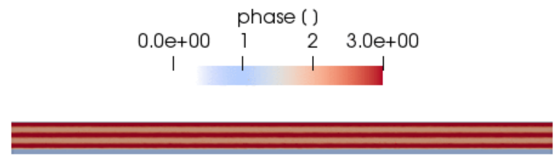
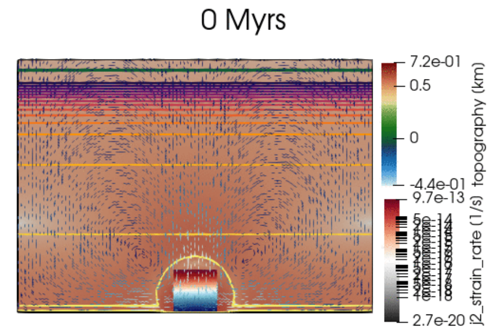
Objective of the course







- Learn how to use a geodynamic modeling code to simulate of wide range of 2D/3D scenario

- To do so, you will use
  - A geodynamic modeling code (LaMEM – 90%)
  - A landscape evolution code (FastScape – 10%)
  - A programming environment (Visual studio)
  - A programming language (Julia)
  - Visualization tools (Paraview, and PlotlyJS (a julia package))
  - A tool to generate density diagram used in LaMEM (MAGEMinApp)

Structure/Organization of the short course

Monday

Morning
- Introduction
- Installation
- First model

Afternoon
- Julia introduction
- Create first setup(s)

Tuesday

Morning
- Building up complexity

Afternoon
- Advanced setup: plume

Wednesday

Morning
- Fold and thrust

Afternoon
- Rifting
- GeophysicalModelGenerator

Thursday

Morning
- Landscape evolution modelling

Afternoon
- Advanced setup: subduction

Friday

Morning and afternoon
- build your own setup

Some tips (based on experience)

- Nothing we are going to do is "complicated" <u>on its own</u>
  - *You don't need advanced mathematical background*
  - *Programming experience will help but is not necessary,*
  - *Copy and paste and modify as much as possible!*

- Complexity arises from chaining several simple tasks

- If you don't do it yourself, you are not going to learn
  - *There is not way around having bugs and solving them*

- When there is a bug, try to understand the error message
  - *Start at the beginning of the error message!*
  - *If this still does not help, try to come back to a working version*
  - *Ask for help!*

- Spend a bit of time making your scripts readable for you
  - *Making it look good helps*
  - *Adding comments is important*

- Modeling is like Lego: you can do a lot, but you are constrained by the building blocks!

Some tips (based on experience)

- Use ChatGPT when you get stuck for common task.
  Mind that ChatGPT is nothing more than a complex interpolation. If there are a lot of data, the answer may be useful

You

given a 3D array Z, write a julia script that extract all the values > 2

ChatGPT

Certainly! Below is the Julia script to extract all the values greater than 2 from a 3D array:

julia — Copy code

```julia
function extract_values_gt_2(arr::Array{Float64, 3})
    return arr[arr .> 2]
end

# Example usage:
# Define a 3D array
Z = rand(-5:5, 3, 3, 3)

# Extract values greater than 2
result = extract_values_gt_2(Z)

println("Values greater than 2 in the 3D array:")
println(result)
```

In this script, `extract_values_gt_2` is a function that takes a 3D array `arr` as input and returns an array containing all the values greater than 2. The `arr .> 2` statement creates a boolean mask indicating which elements of `arr` are greater than 2. This mask is then used to extract the desired values from the original array. Finally, we print the extracted values.

This is how to do!

Mostly useless

Some tips (based on experience)

- Once you have a prompt that is useful update it

For instance:

You

let's say that I now want to extract all the values > 2, and smaller than 3.6, update the script

ChatGPT

Sure, you can modify the script to extract values greater than 2 and smaller than 3.6 using logical operators. Here's the updated script:

julia — Copy code

```julia
function extract_values_between_2_and_3_6(arr::Array{Float64, 3})
    return arr[(arr .> 2) .& (arr .< 3.6)]
end

# Example usage:
# Define a 3D array
Z = rand(-5:5, 3, 3, 3)

# Extract values between 2 and 3.6
result = extract_values_between_2_and_3_6(Z)

println("Values between 2 and 3.6 in the 3D array:")
println(result)
```

This is how to do!

Mostly useless

In this modified version, the function `extract_values_between_2_and_3_6` now returns values that satisfy both conditions: greater than 2 and smaller than 3.6. The logical operator `.&` is used to perform element-wise AND operation between the boolean arrays generated by the conditions `arr .> 2` and `arr .< 3.6`. This ensures that only elements that satisfy both conditions are selected.

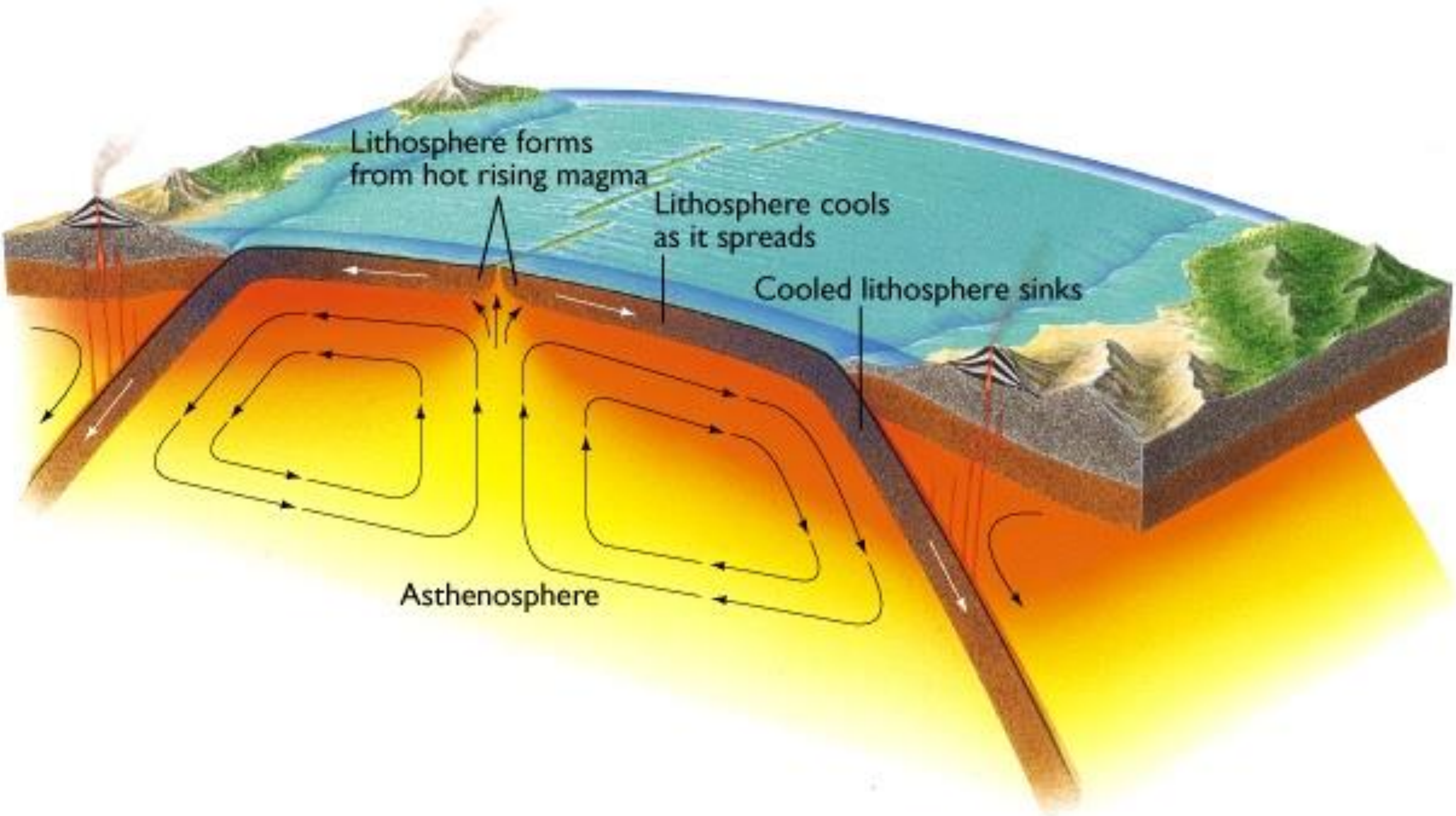
Very useful

LaMEM

Lithosphere and Mantle Evolution Model

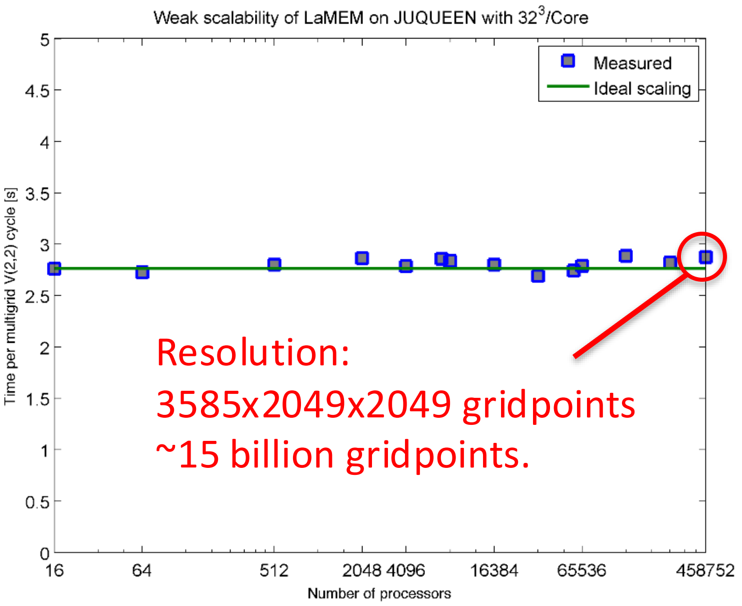
General overview

Geodynamic modelling



What is LaMEM?

- **L**ithosphere **a**nd **M**antle **E**volution **M**odel
- 3D thermo-mechanical code, written in C/PETSc.
- Nonlinear visco-elasto-visco-plastic rheologies
- MPI-parallel; runs on 1-458’752 processors.
- Staggered finite difference method (faster than FEM).
- Can use a large variety of (multigrid) solvers (Galerkin GMG, AMG, Coupled/decoupled)
- Marker-and-cell method, free surface, (coupled to simple erosion model).
- Phase transitions
- Polygonal meshes (geomIO) to create (complex) 3D input geometries.



Equations

$$\frac{\partial u_i}{\partial x_i} = -\frac{1}{K}\cdot\frac{dP}{dt}$$ conservation of mass

$$-\rho g_i = -\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}$$ conservation of momentum

$$\dot{\varepsilon}_{ij} = \frac{1}{2\eta_{eff}}\tau_{ij} + \frac{1}{2G}\frac{D\tau_{ij}}{Dt} + \dot{\lambda}\frac{\partial Q}{\partial \sigma_{ij}}$$ visco-elasto-plastic rheology

$$\rho c \frac{DT}{Dt} = \frac{\partial}{\partial x_i}\left(k\frac{\partial T}{\partial x_i}\right) + H_{sources}$$ conservation of energy

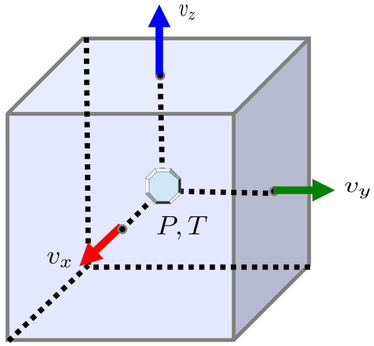
"Stokes" flow

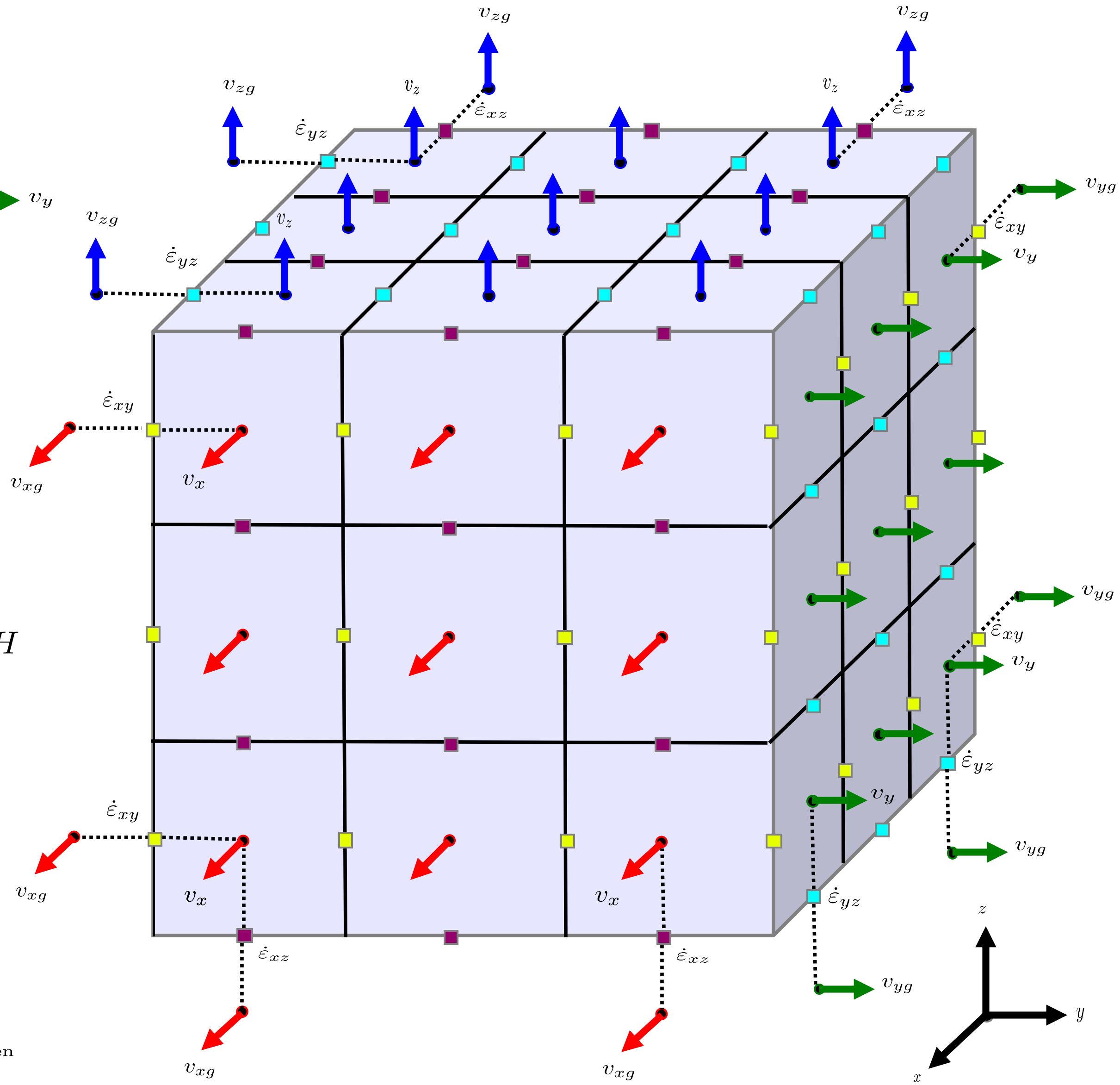
$$\frac{\partial u_i}{\partial x_i} = 0$$

$$-\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\eta_{eff}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right) = -\rho g_i \longrightarrow \begin{pmatrix} \mathbf{K} & \mathbf{G} \\ \mathbf{G}^{\mathbf{T}} & \mathbf{0} \end{pmatrix}\begin{pmatrix} \mathbf{u} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ \mathbf{g} \end{pmatrix}$$

- Complexities mainly from the nonlinear rheology.
- Typically need to be solved numerically.
- No time derivative in Stokes equations!
  - For given density and viscosity distribution, velocity is given everywhere

Parallel staggered grid layout implementation





Equations:

$$\frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial P}{\partial x_i} + \rho g_i = 0$$

$$\frac{1}{\rho}\frac{D\rho}{Dt} + \frac{\partial v_i}{\partial x_i} = 0$$

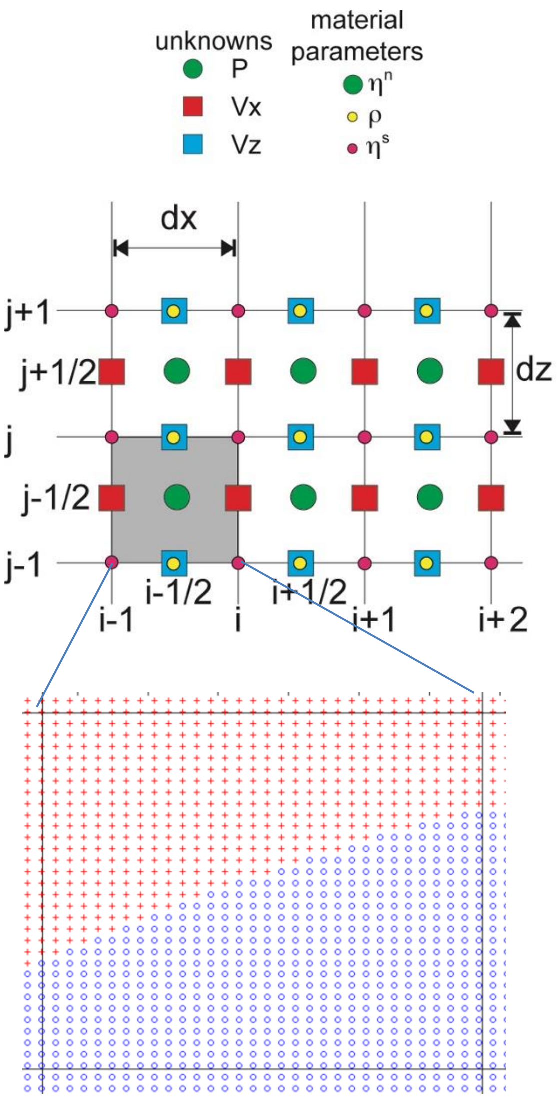
$$\rho C_p \frac{DT}{Dt} = \frac{\partial}{\partial x_i}\left(\lambda \frac{\partial T}{\partial x_i}\right) + H$$

Legend:

- v_x, q_x
- v_y, q_y
- v_z, q_z
- $\dot{\varepsilon}_{xy}, \tau_{xy}, \eta_{xy}$
- $\dot{\varepsilon}_{xz}, \tau_{xz}, \eta_{xz}$
- $\dot{\varepsilon}_{yz}, \tau_{yz}, \eta_{yz}$
- $P, \dot{\varepsilon}_{xx}, \dot{\varepsilon}_{yy}, \dot{\varepsilon}_{zz}$
  $\tau_{xx}, \tau_{yy}, \tau_{zz}, \eta_{\text{cen}}$
  T, ρ, C_p, λ, H

Marker & Cell approach

- Rock types are tracked by markers (called “Particles” in LaMEM).
- Each particle:
  - Is of a certain rocktype (or “phase ID”)
  - Contains info such as temperature, stress etc.
- Are advected with the flow
- During every timestep, the particles are mapped back to the computational grid, and vice versa



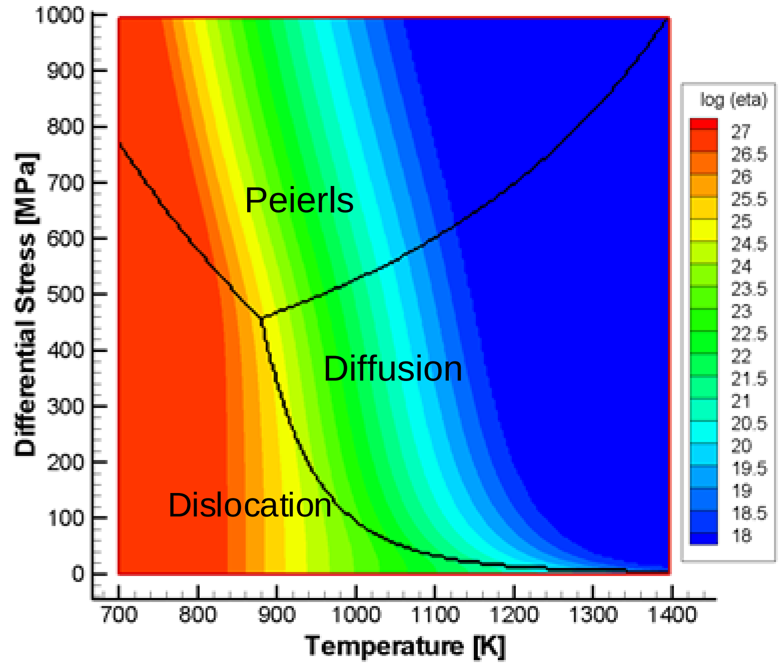
Nonlinear visco-elasto-plastic rheology

Drucker-Prager yield stress (brittle faulting)

$$\tau_Y = \mu P + c$$

Diffusion, Dislocation and Peierls creep

$$A_l = B_l \ \exp\left[-\frac{E_l + pV_l}{RT}\right],$$
$$A_n = B_n \ \exp\left[-\frac{E_n + pV_n}{RT}\right]$$
$$A_p = \frac{B_p}{(\gamma\tau_p)^s} \ \exp\left[-\frac{E_p + pV_p}{RT}(1-\gamma)^q\right]$$



Effective creep viscosities

$$\begin{aligned}
\eta_l &= \frac{1}{2}\left(A_l\right)^{-1} \\
\eta_n &= \frac{1}{2}\left(A_n\right)^{-\frac{1}{n}}\left(\dot{\varepsilon}^*_{II}\right)^{\frac{1}{n}-1} \\
\eta_p &= \frac{1}{2}\left(A_p\right)^{-\frac{1}{s}}\left(\dot{\varepsilon}^*_{II}\right)^{\frac{1}{s}-1}
\end{aligned}$$

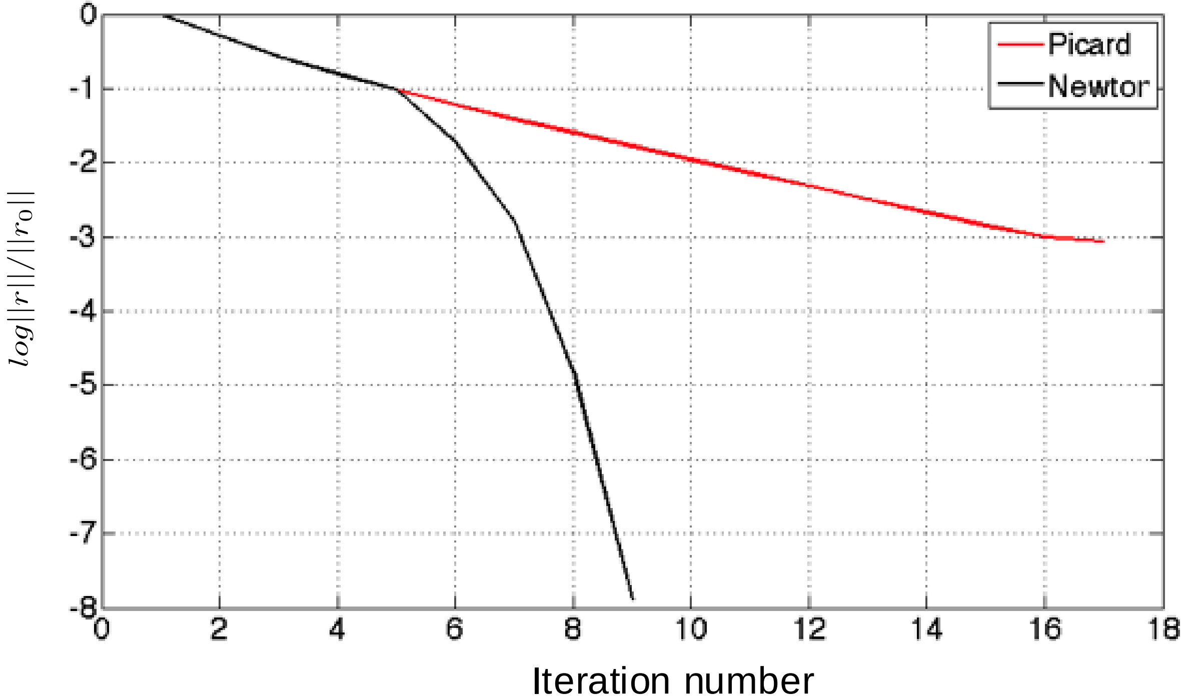
Peierls effective exponent

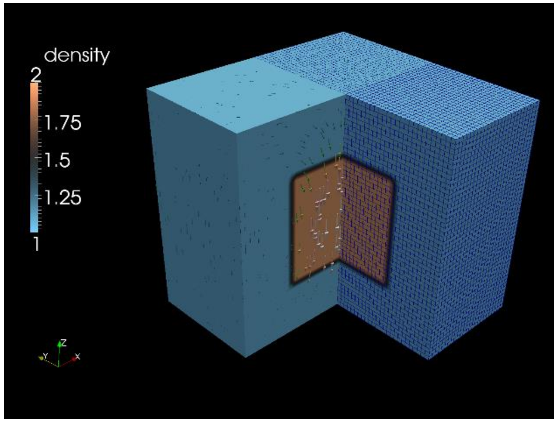
$$s = \frac{E_p + PV_p}{RT}(1-\gamma)^{q-1} \, q \, \gamma$$

Picard vs. Newton

Quasi-linear residual form: $r(x) = A(x)\,x - b = 0$

Picard fixed-point iteration: $J(x) \approx A(x)$

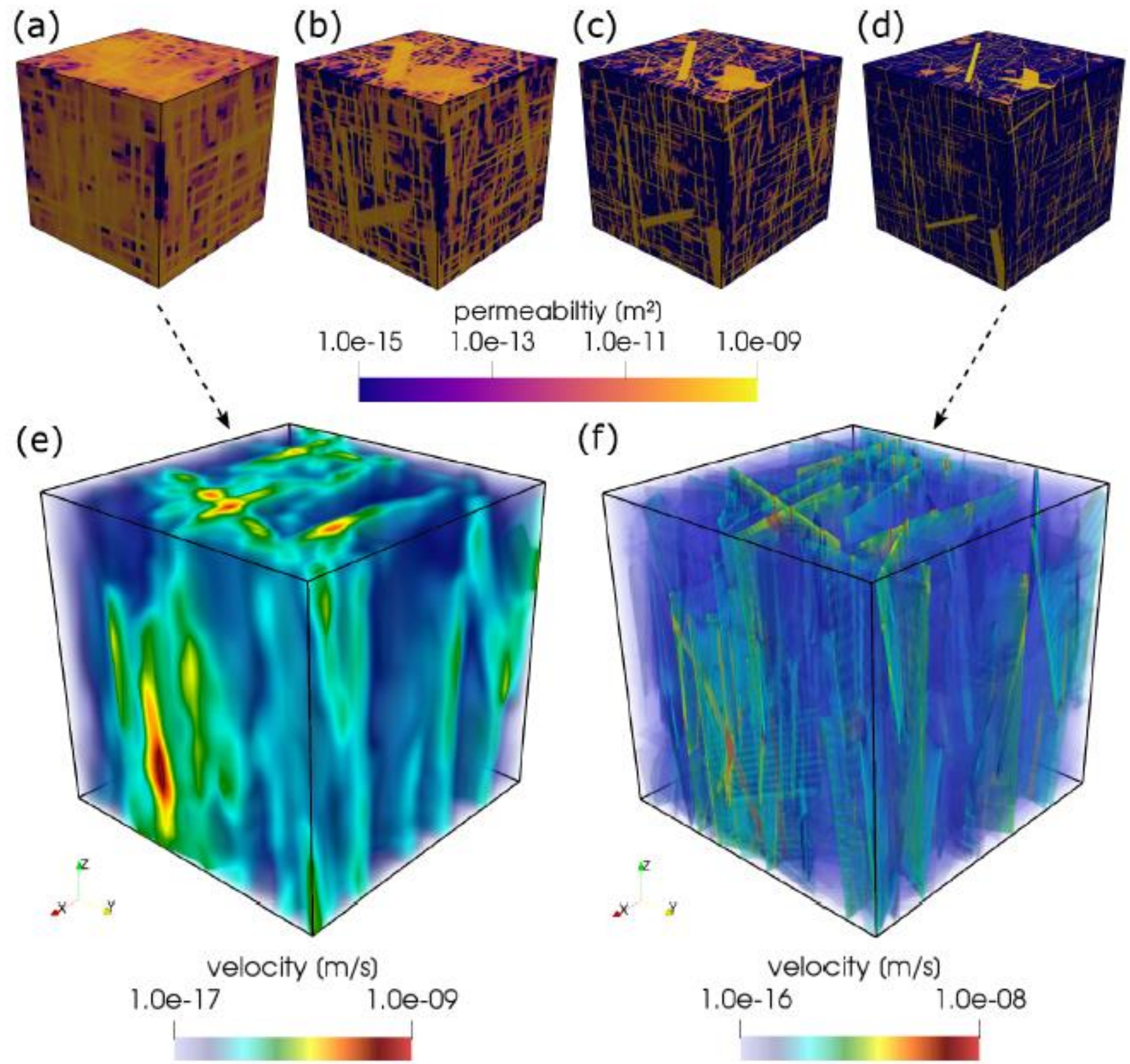




- Newton much faster than Picard for nonlinear materials
- Picard approximation facilitates convergence at the initial stages
- Switching to Picard can improve Newton convergence

Some recent LaMEM applications

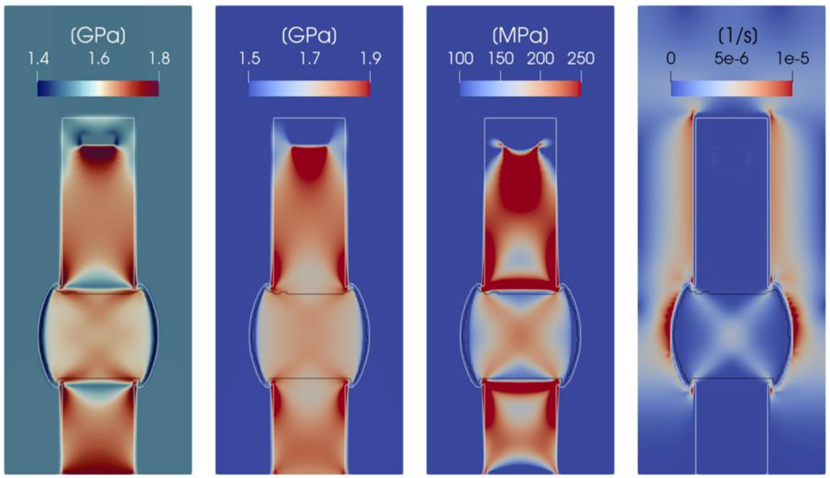
Fracture network permeability study



Kottwitz et al., 2021 – Solid Earth

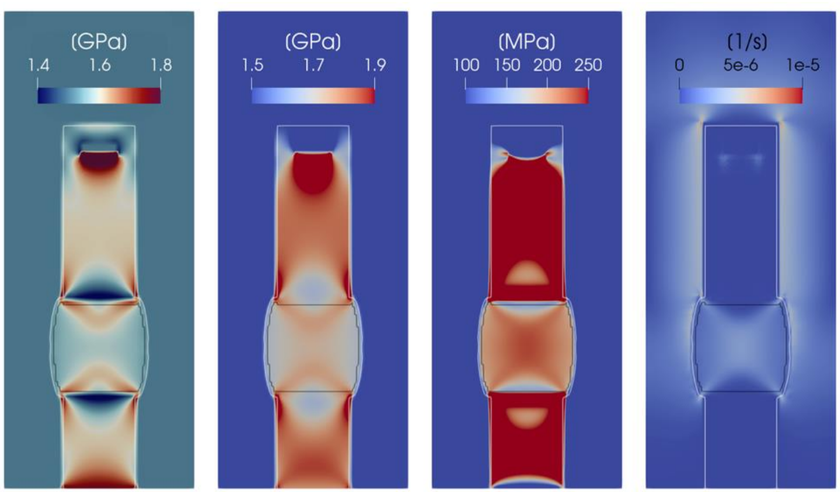
High-pressure rock deformation experiments

2D



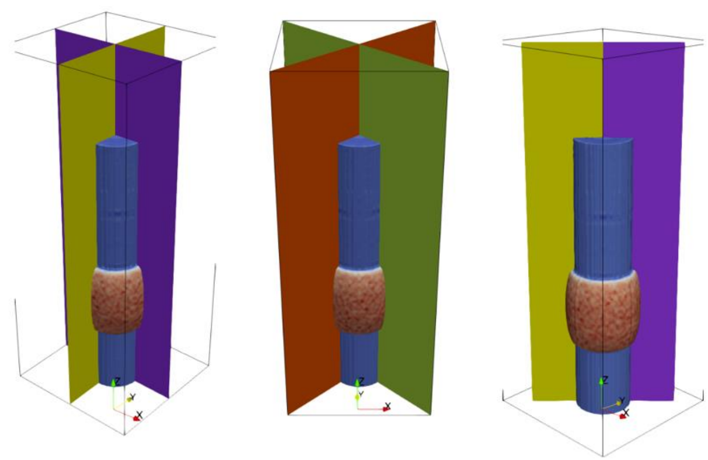
(a) pressure (b) σ_1 (c) $\Delta\sigma$ (d) strain rate

3D



(a) pressure (b) σ_1 (c) $\Delta\sigma$ (d) strain rate

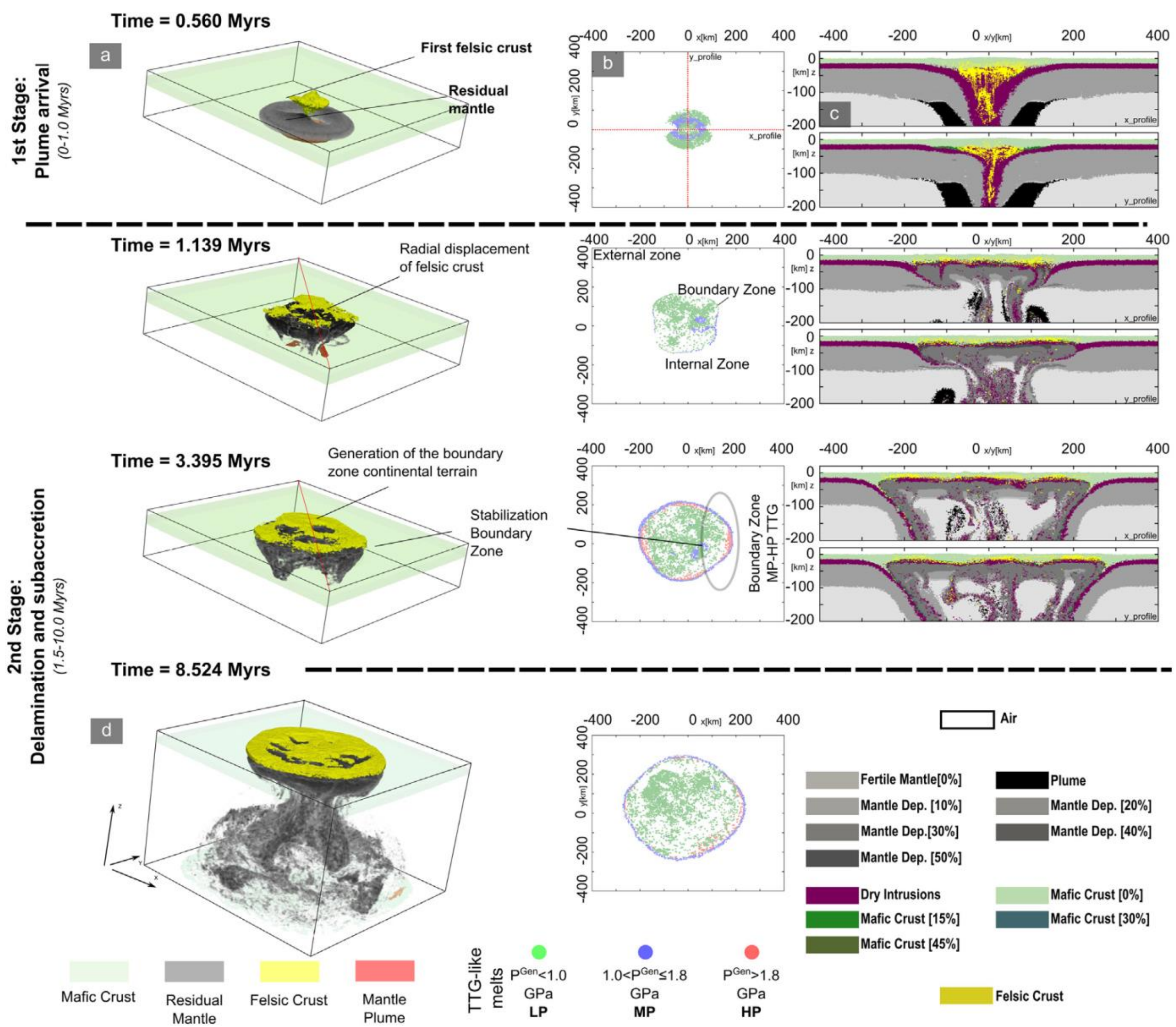
Kilian Herrmanns
(BSc Thesis, Heidelberg)



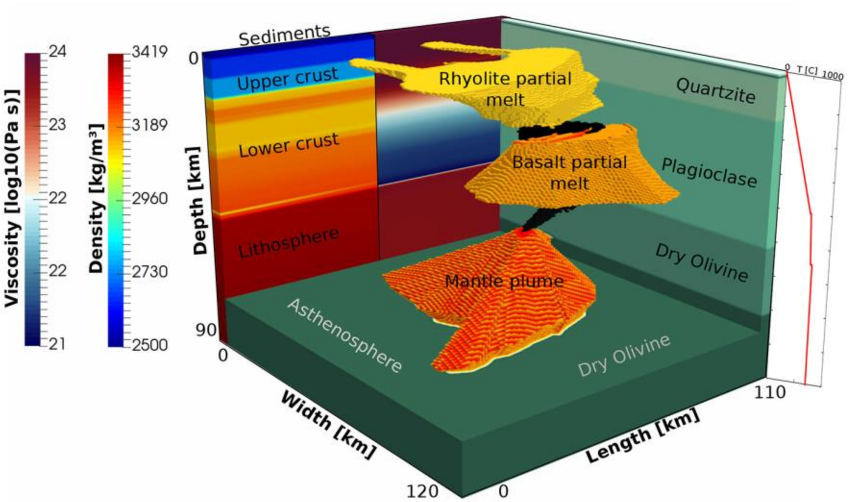
(a) X and Y planes (b) Diagonal planes [110] and [-110] (c) Display of plane orientation for A6

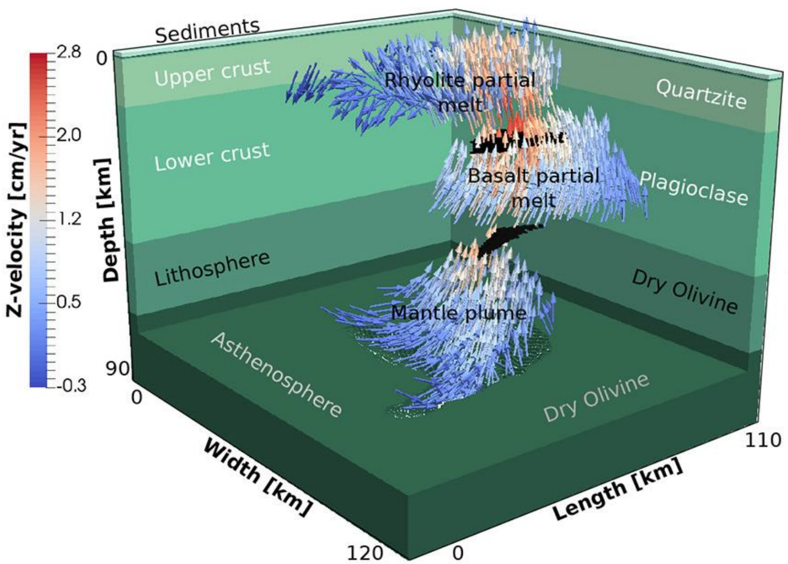
Plume - LID interaction during the Archean

Piccolo et al., 2020 – Gondwana research

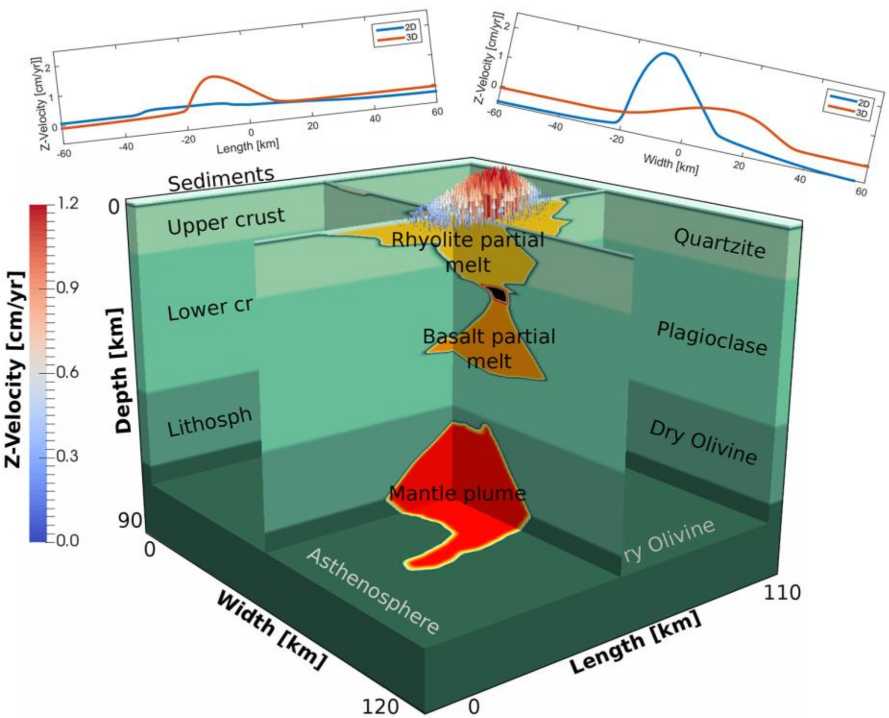


Yellowstone Magmatic System



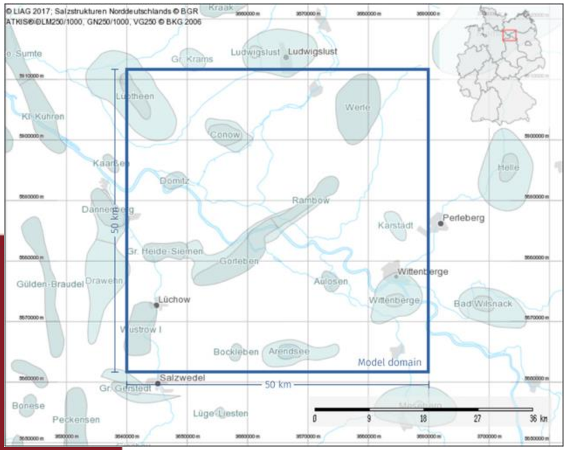


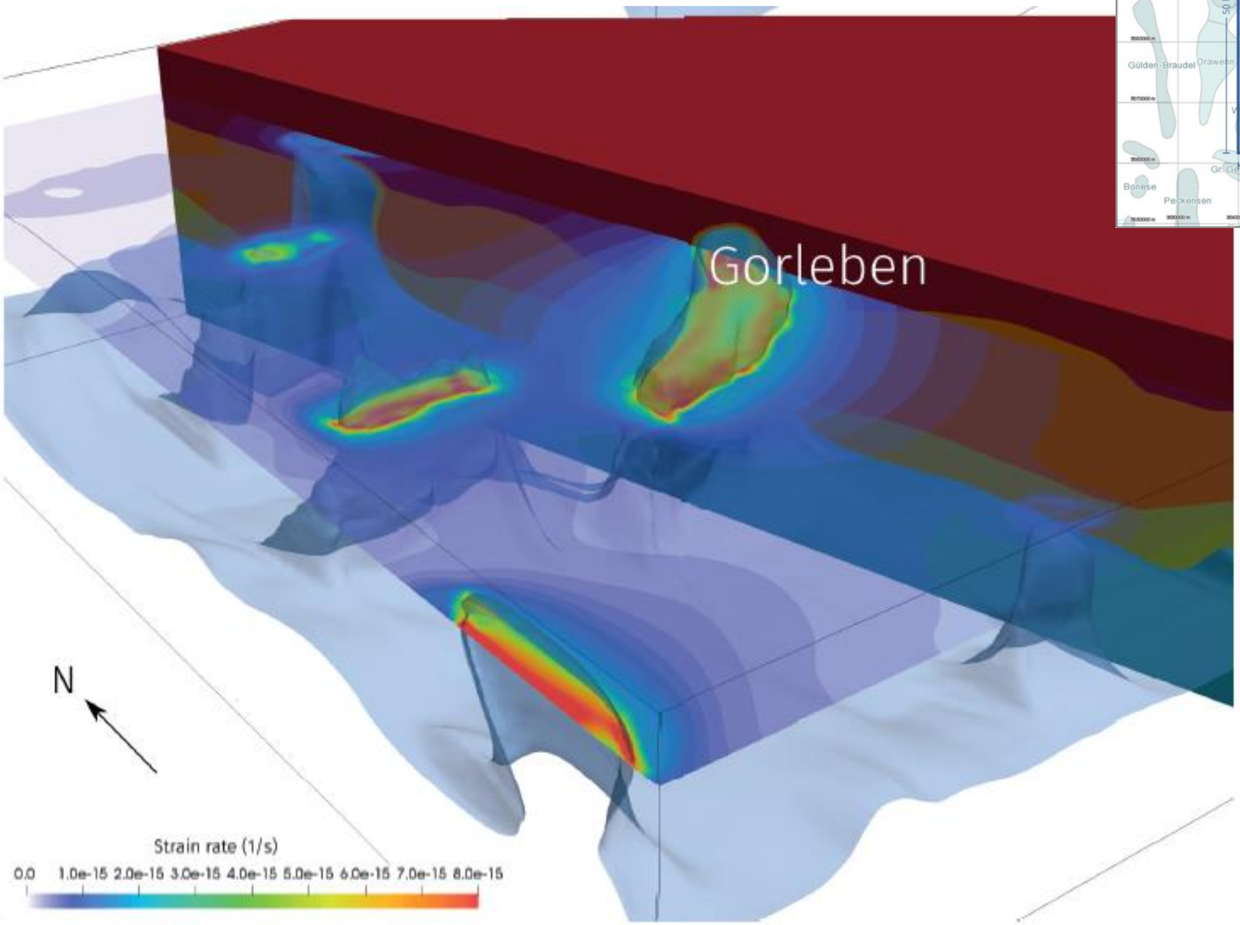
Reuber et al., 2018, Frontiers in Earth Sciences



Gorleben salt dome

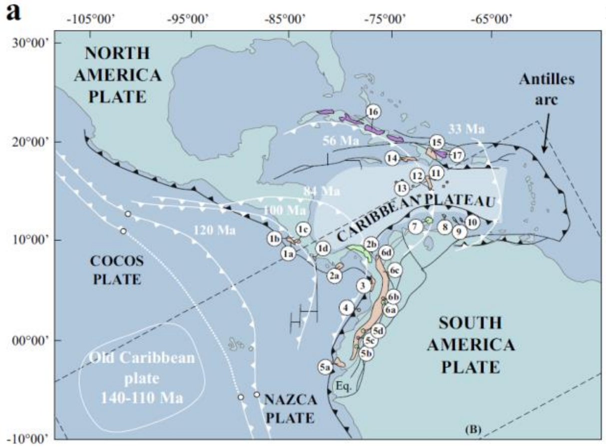
- Salt cavities as potential storage of radioactive waste?

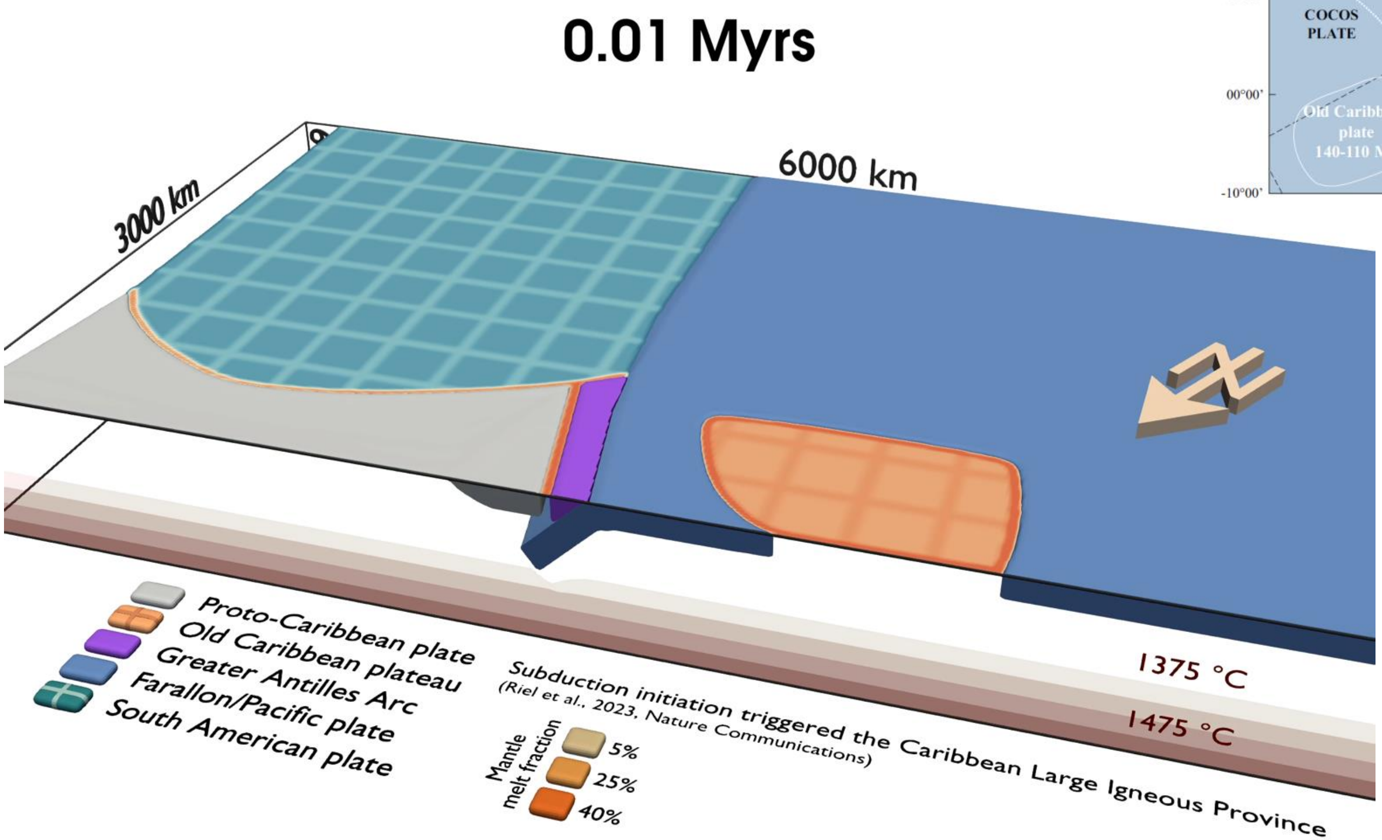




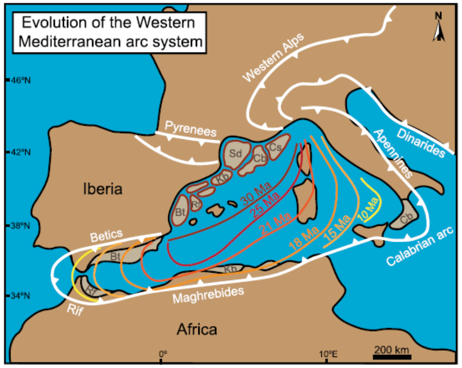
Baumann et al., 2018

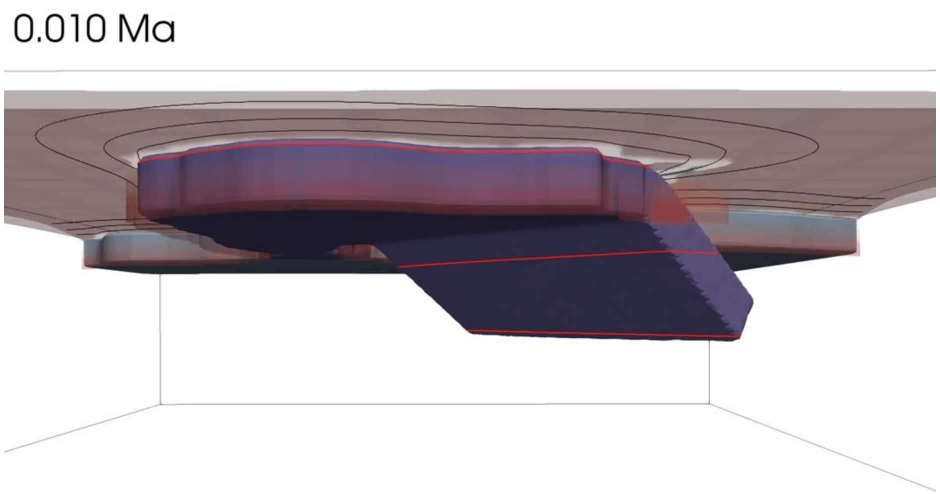
Formation of Caribbean LIP

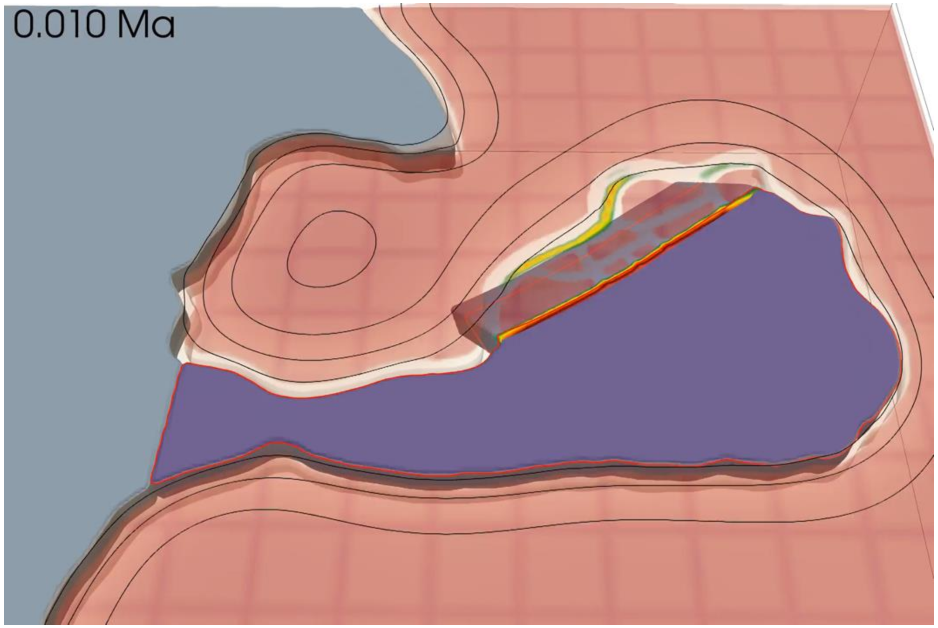




Subduction invasion - Gibraltar

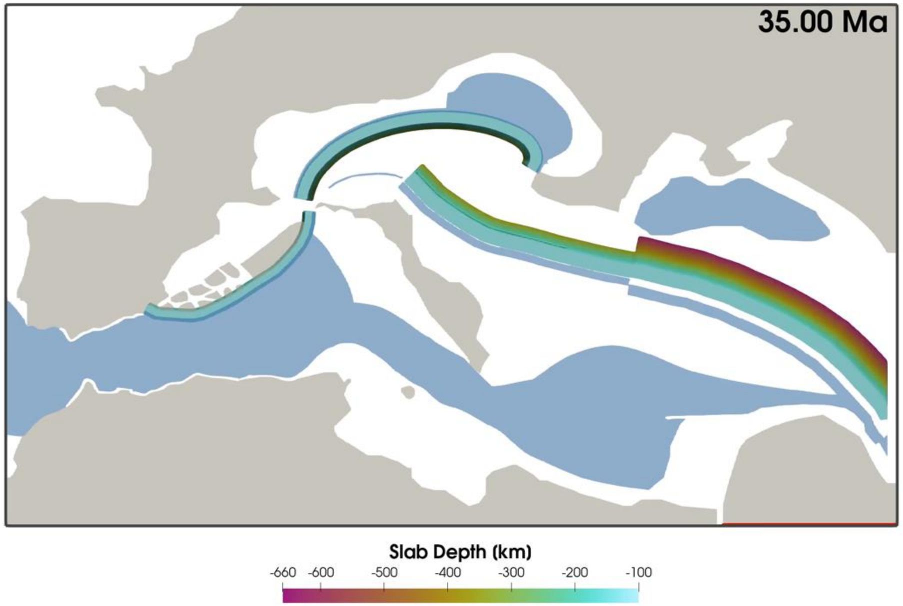


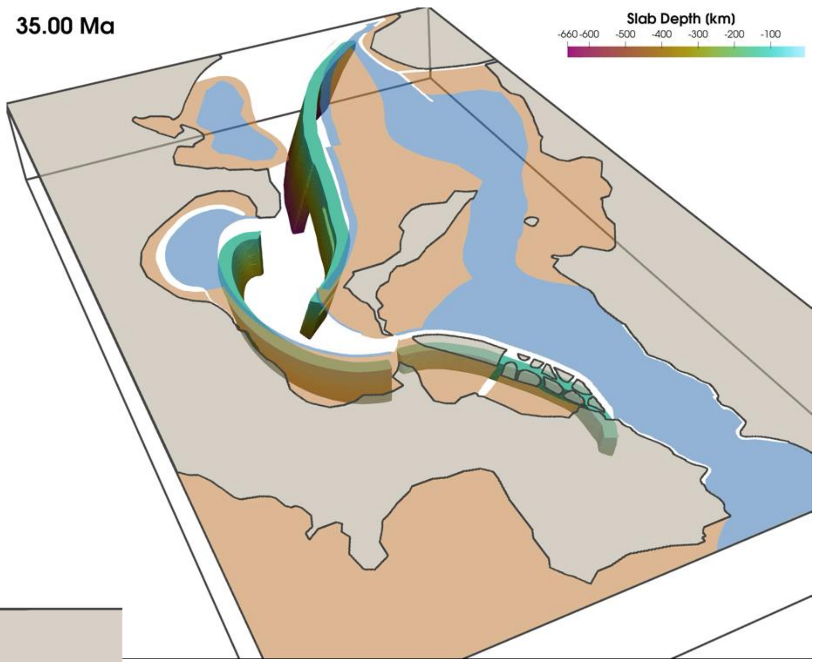


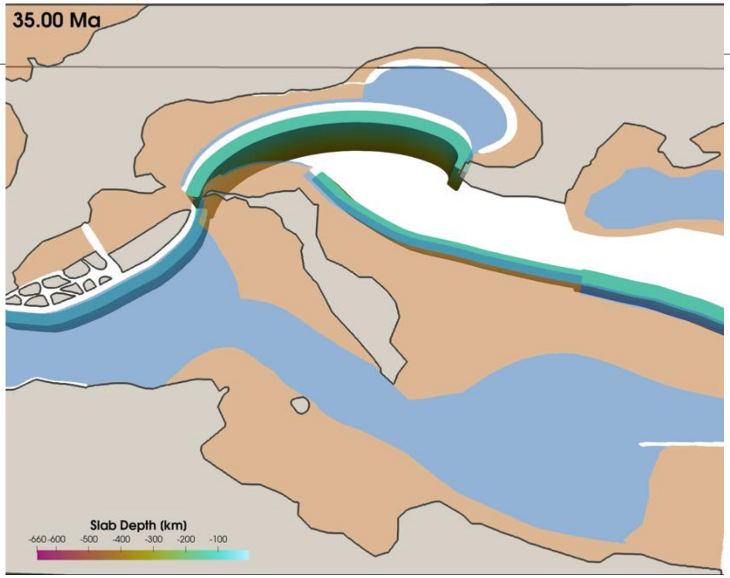


Duarte, Riel et al ., 2024 – Geology

Mantle Dynamics in the Mediterranean and Plate Motion of the Adriatic Microplate



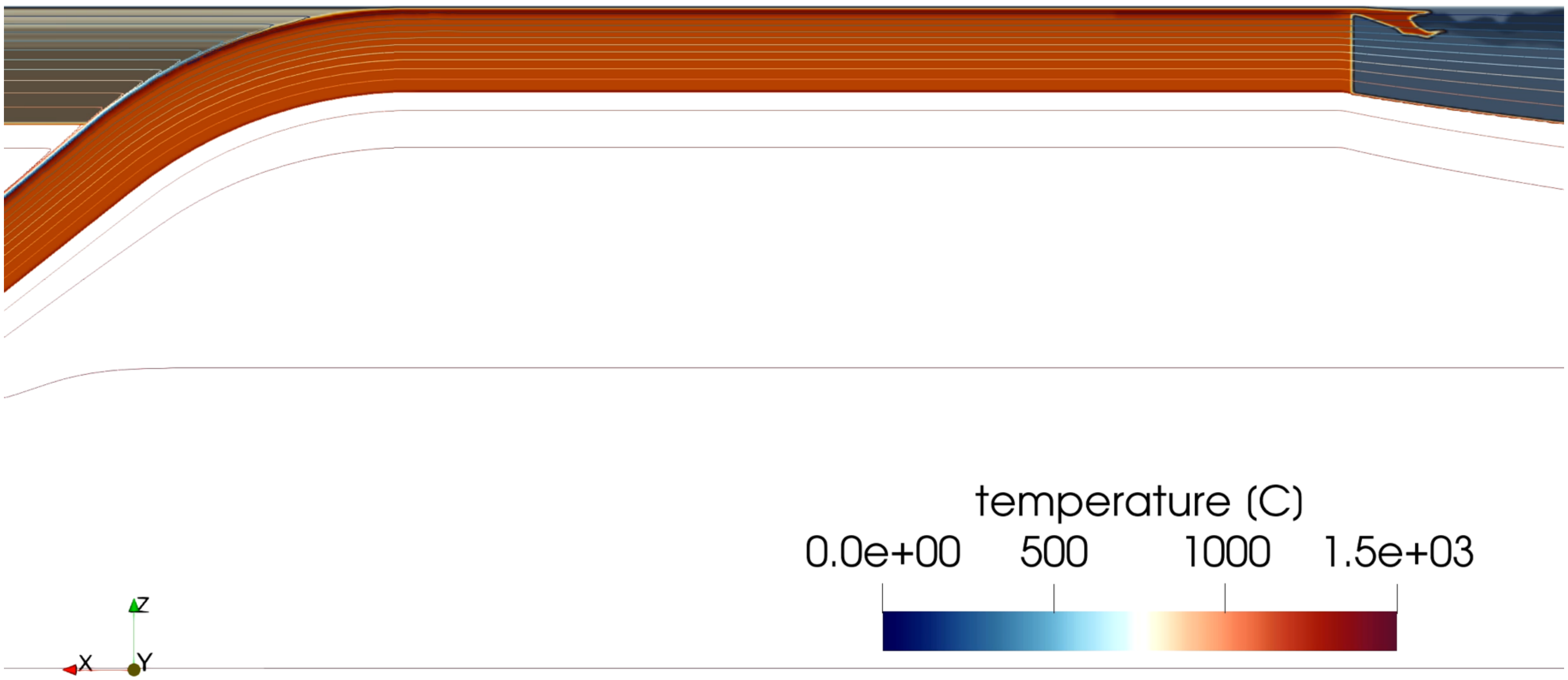




Schuler et al., 2025 G-cubed

Role of lower crust in Orogen build-up

Rodrigues et al, in prep



Ridge opening and mantle window

Rojas-Agramonte, to be submitted