Using deal.II's particle infrastructure to improve models of transient geodynamic processes

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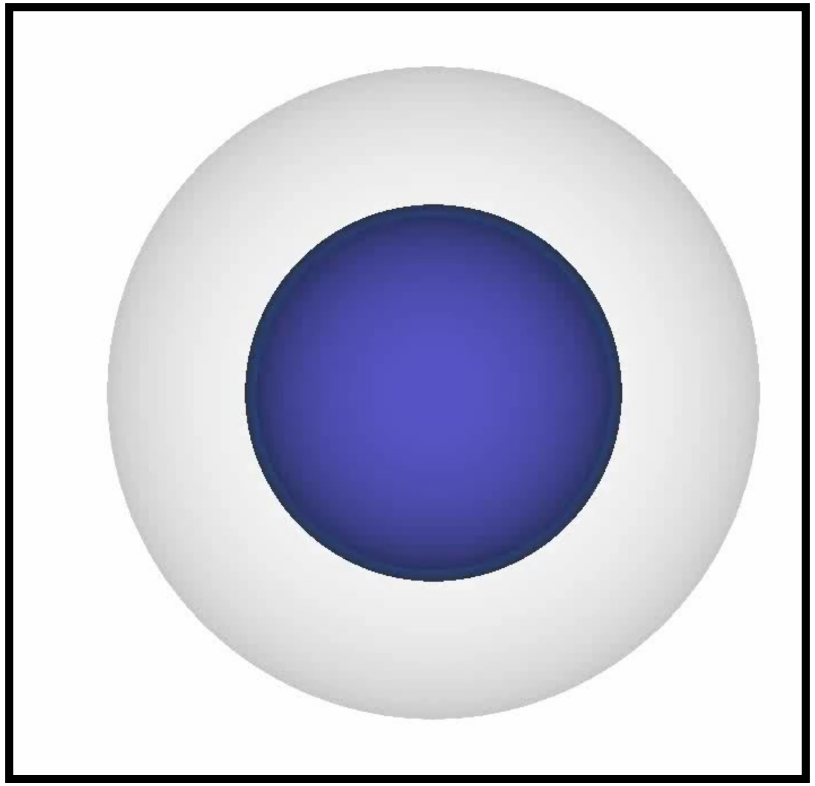
with work by: Juliane Dannberg, Wolfgang Bangerth, Gerry Puckett, Cedric Thieulot, Timo Heister
Josh Russel, Zach Eilon, Menno Fraters, Ranpeng Li, Arushi Saxena, Bob Myhill, Dan Thallner

- Observational Data
- Numerical models
- Computational Infrastructure



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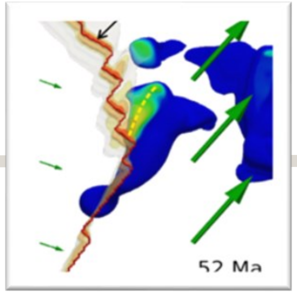
COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

ASPECT

deal.II

PREVIOUS WORK

ASPECT



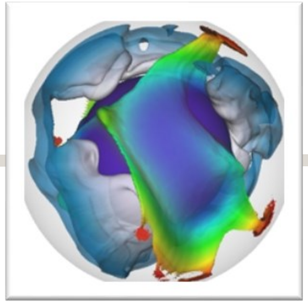
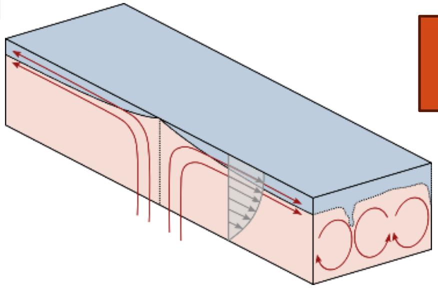
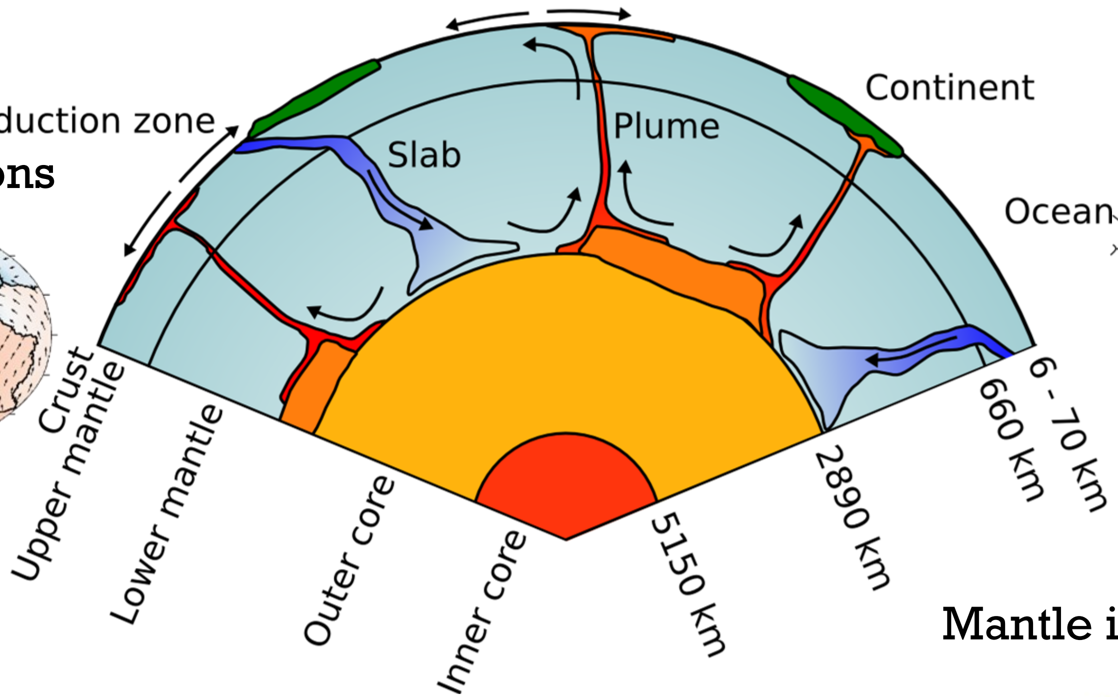


Plate-LLSVP interaction

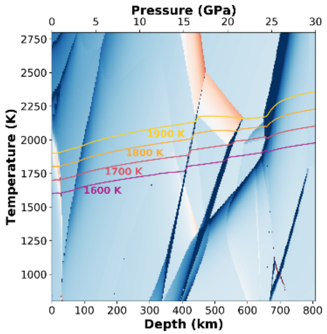


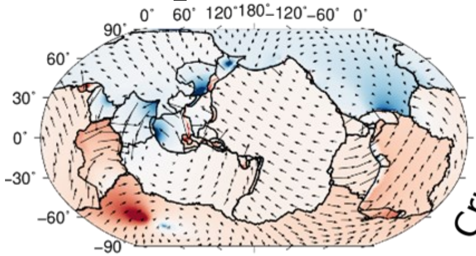
Small-scale convection

Plume-ridge interaction

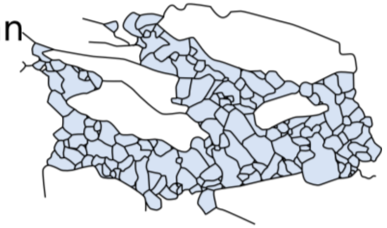


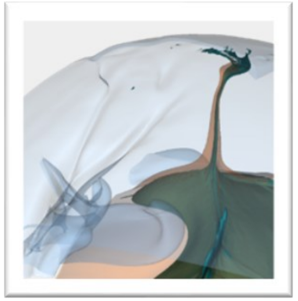
Global plate motions





Grain-size evolution

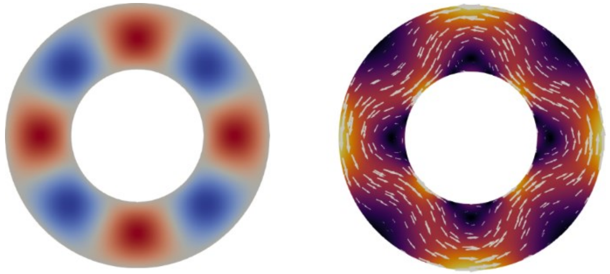


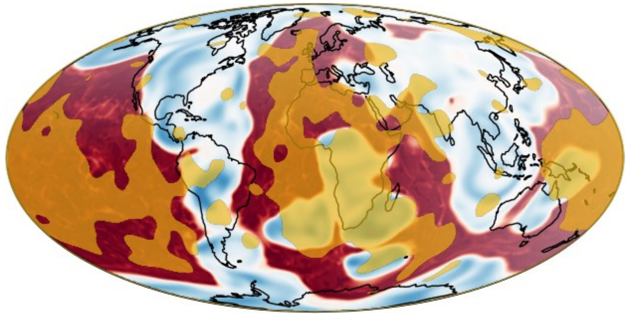


Plume locations and zonation

Mantle phase transitions

Mantle influence on geodynamo





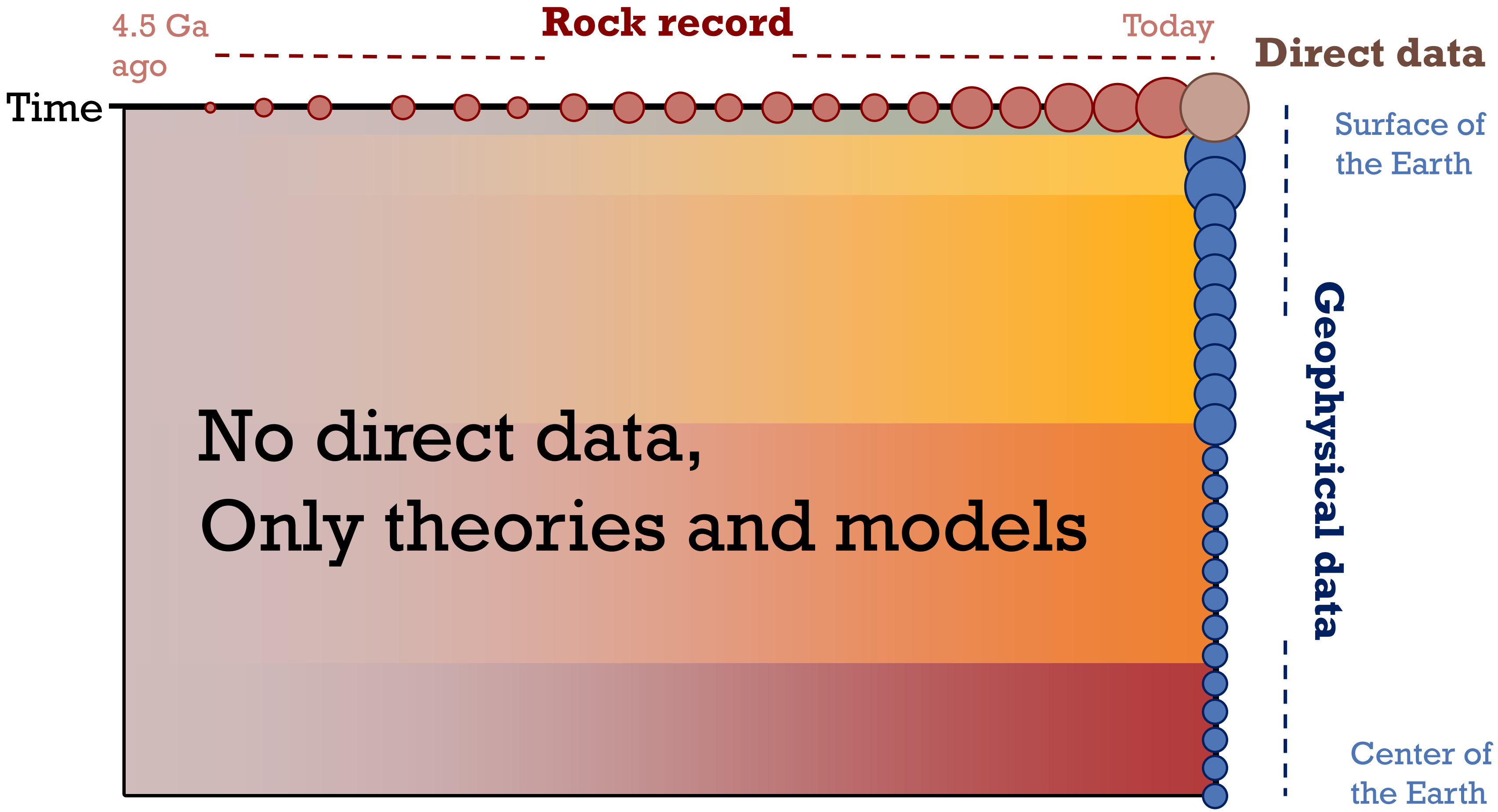
Benchmarking geodynamic models

WHY GEODYNAMIC MODELING?

- Many features on the Earth's surface can only be understood through their connection with processes in the Earth's interior.

- Problem:
The Earth's interior is largely inaccessible.

Available observations:

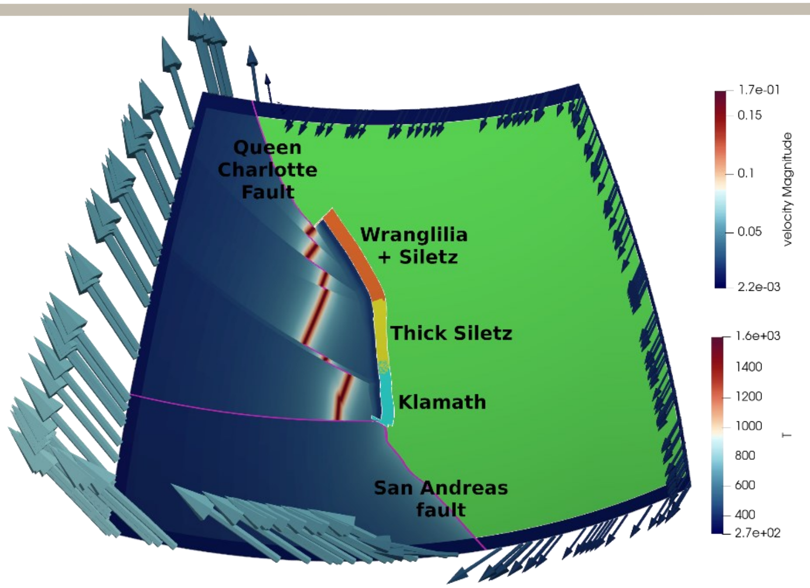


After Gerya, 2014

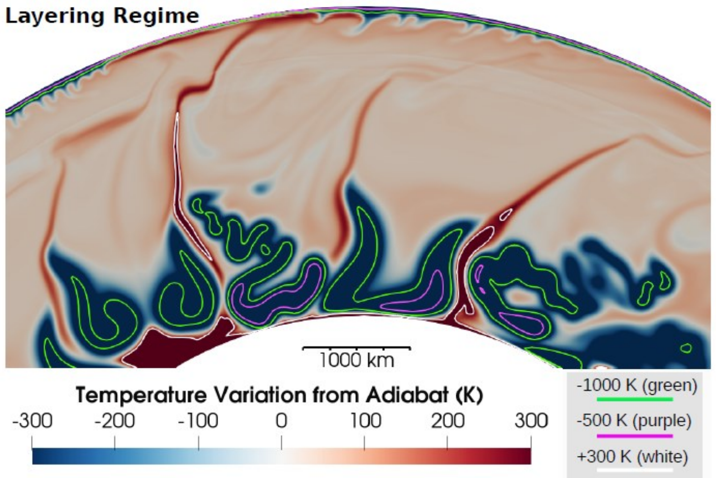
MODEL TYPES

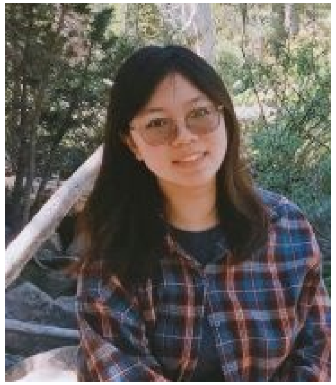
- **Specific Modeling:**
  Attempts to reproduce the specific state of a certain geodynamic system (e.g. based on a specific observation) to better understand that state.

- **Generic modelling:**
  Attempts to produce different regimes of behavior of a certain geodynamic system (e.g. based on a general observation) to better understand the processes.



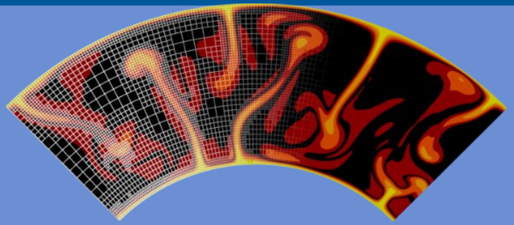
Menno Fraters et al., in prep.





Ranpeng Li et al., in review.

Benchmarking the accuracy and performance of particle methods in ASPECT/deal.II



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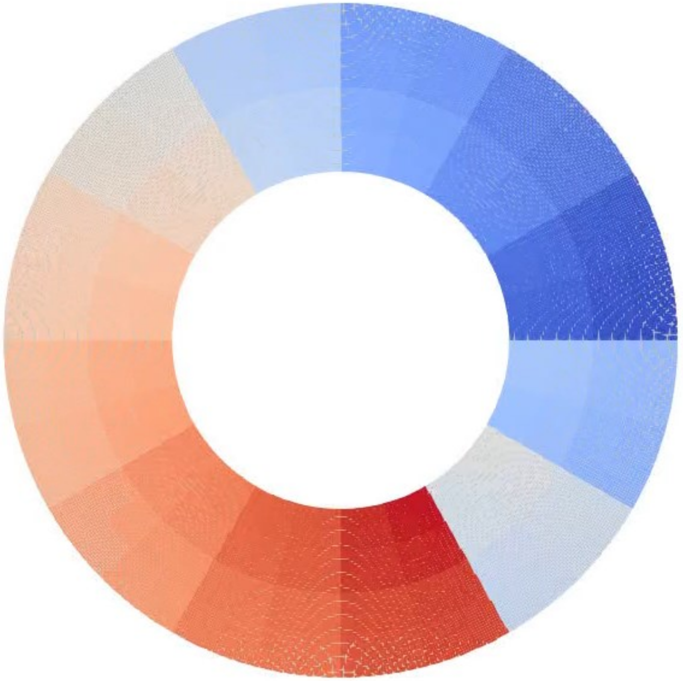
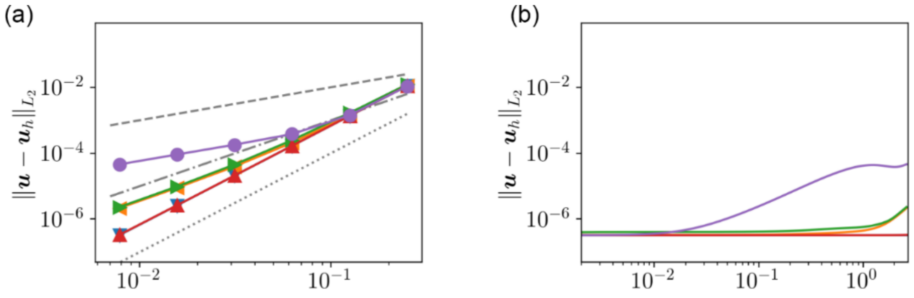


$$-\Delta \boldsymbol{u} + \nabla p = \rho \boldsymbol{g}, \qquad (1)$$

$$\nabla \cdot \boldsymbol{u} = 0. \qquad (2)$$

$$\frac{\partial q}{\partial t} + \mathbf{u} \cdot \nabla q - \nabla \cdot (D \nabla q) = 0 \qquad (3)$$



COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

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BENCHMARKING GEODYNAMIC MODELS

- Based on physical first principles
- Governing equations:
  - Force balance (1)
  - Mass conservation (2)
  - Conservation of energy or composition (3)

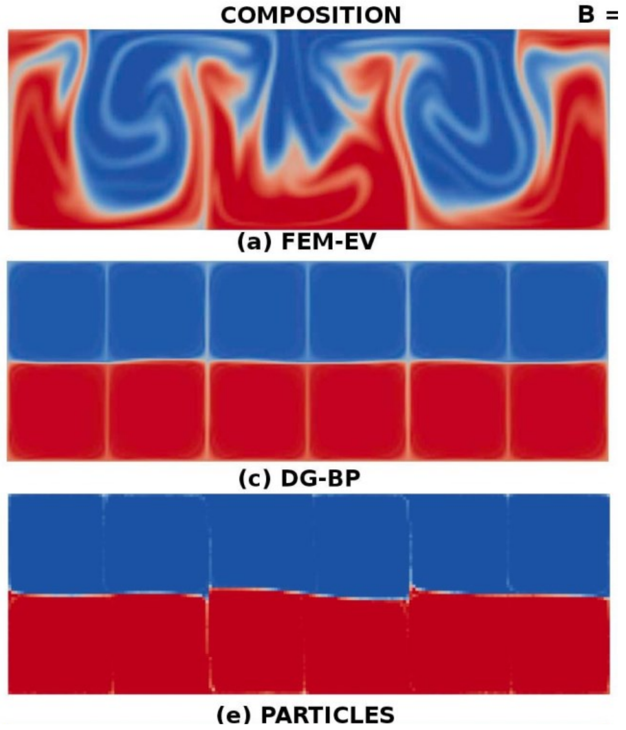
  Force balance (1) and Mass conservation (2): Stokes equations
- Stokes equations solved using finite-element method
- (3) solved using FEM, or particles(/tracers)

- Benchmarking allows to check if solution method is correct
- Benchmarking allows to pick an appropriate solution method

$$-\Delta \boldsymbol{u} + \nabla p = \rho \boldsymbol{g}, \qquad (1)$$

$$\nabla \cdot \boldsymbol{u} = 0. \qquad (2)$$

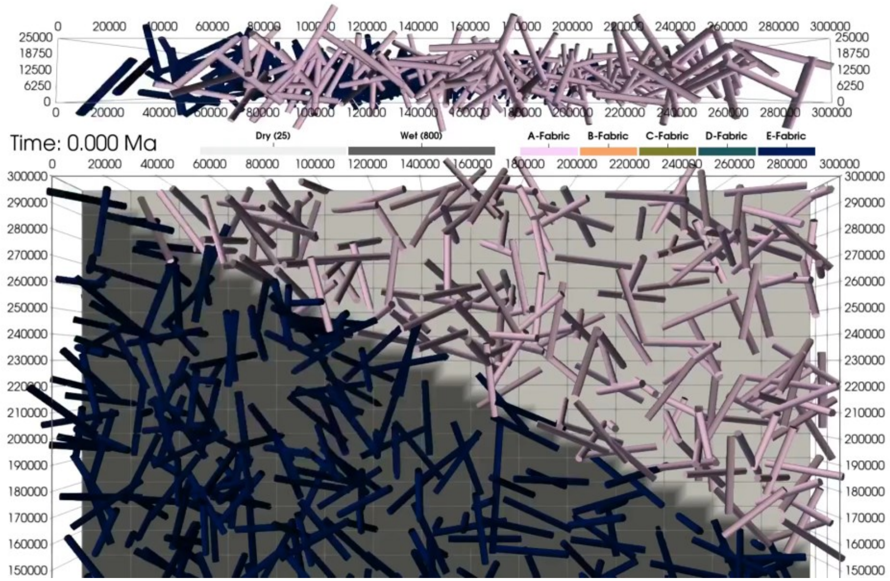
$$\frac{\partial q}{\partial t} + \mathbf{u} \cdot \nabla q - \nabla \cdot (D \nabla q) = 0 \qquad (3)$$



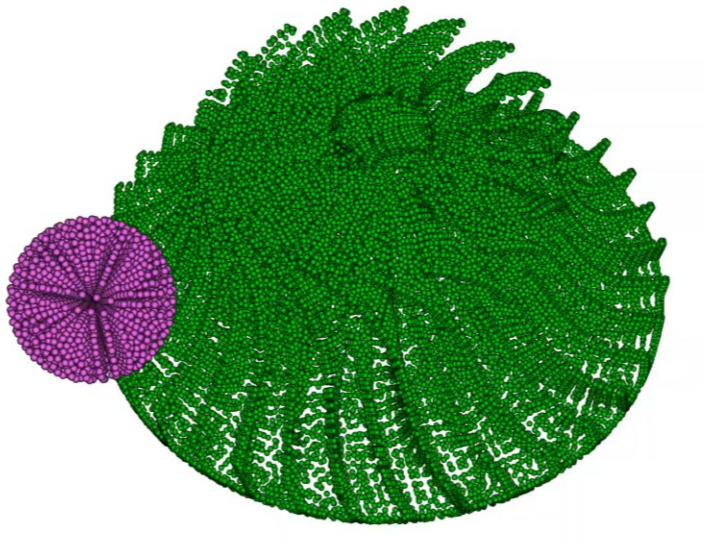
Puckett et al., 2018

A FLEXIBLE PARTICLE FRAMEWORK

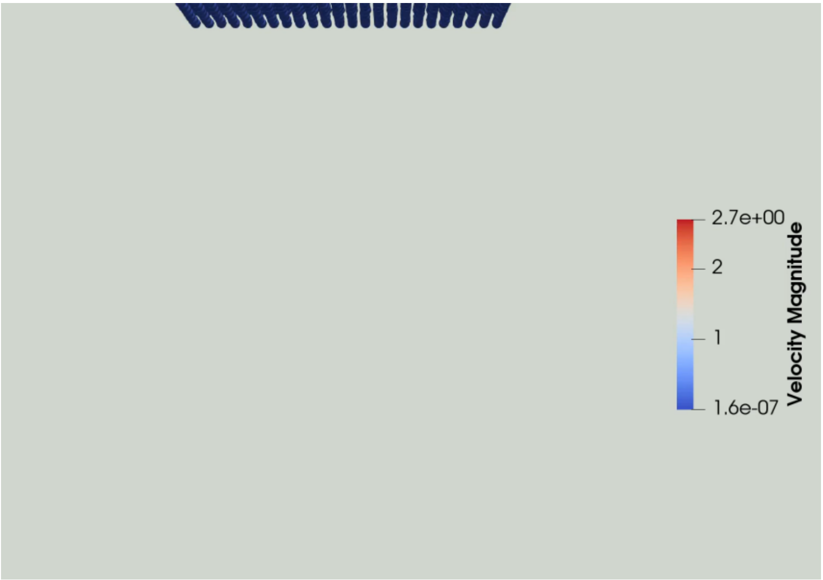
- Past work: Application agnostic software infrastructure for particles
- Arbitrary, higher-order (e.g. curved) geometry, adaptively refined and changing meshes
- Accuracy, flexibility and scalability of our particle software infrastructure (Gassmöller et al., 2017, 2019, 2024, Arndt et al. 2021, Golshan et al. 2022)



Crystal-preferred orientation in corner flow, Fraters & Billen, 2021



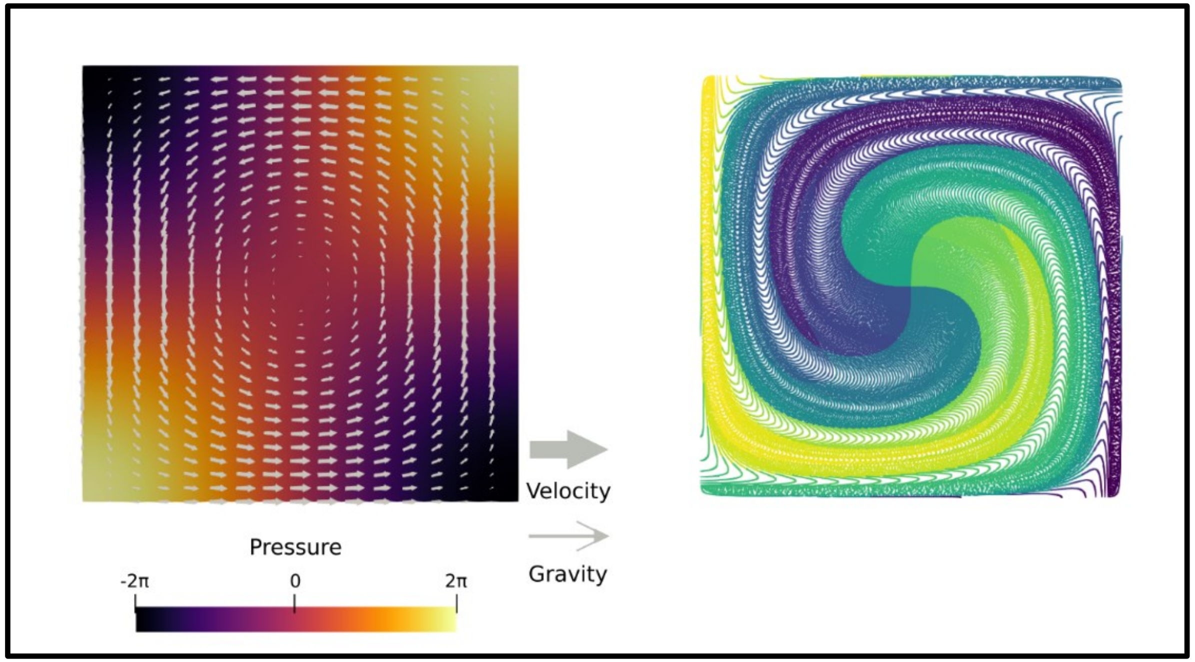
Fluid-Structure Interaction, 3D impeller, deal.II Step 70, Luca Heltai



Filling of a silo, Lethe-DEM, Golshan et al., 2022

METHOD OF MANUFACTURED SOLUTIONS

- Know the equations to solve, e.g. Stokes equations:
- "Manufacture" solutions for these equations, set the parameters to fulfil solutions



$$-\Delta \boldsymbol{u} + \nabla p = \rho \boldsymbol{g},$$
$$\nabla \cdot \boldsymbol{u} = 0.$$

$$\boldsymbol{u} = \begin{bmatrix} \sin(\pi x)\cos(\pi y) \\ -\cos(\pi x)\sin(\pi y) \end{bmatrix},$$

$$p = 2\pi\cos(\pi x)\cos(\pi y),$$

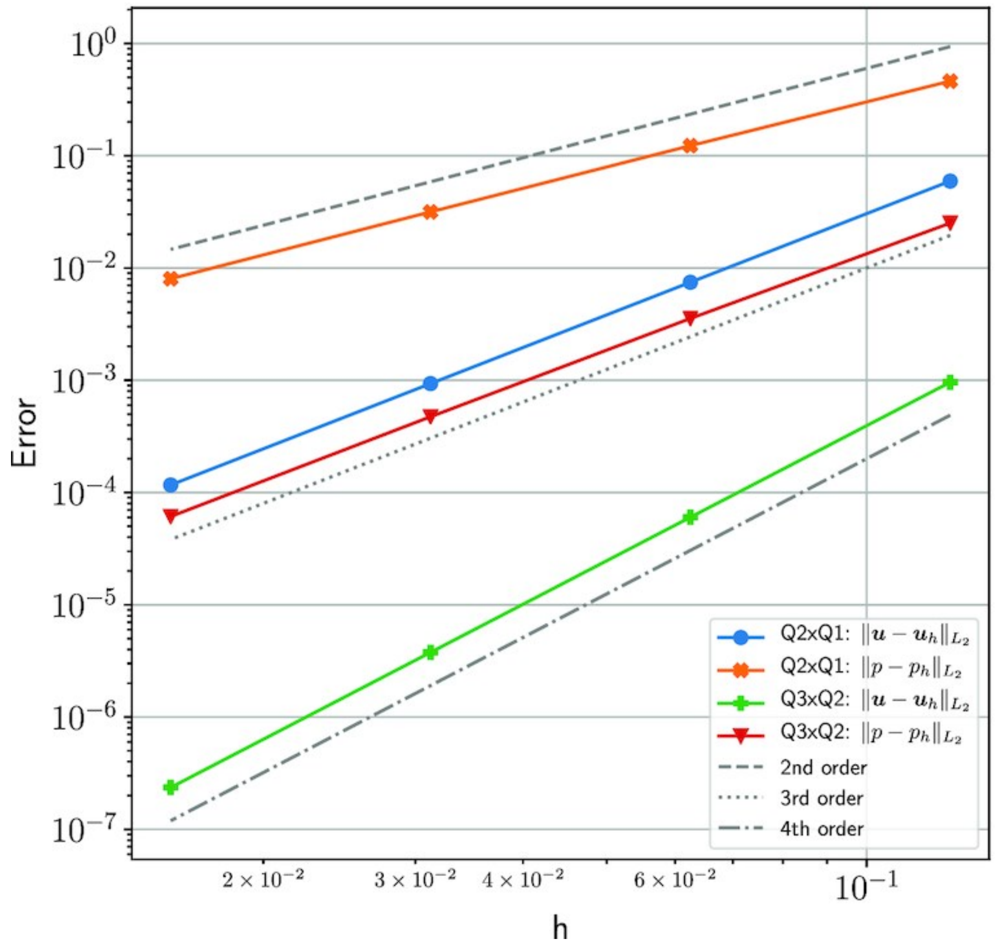
$$\rho = \sin(\pi x)\sin(\pi y),$$

$$\boldsymbol{g} = \begin{bmatrix} 0 \\ -4\pi^2 \frac{\cos(\pi x)}{\sin(\pi x)} \end{bmatrix}.$$

Gassmoeller et al, GJI, 2019

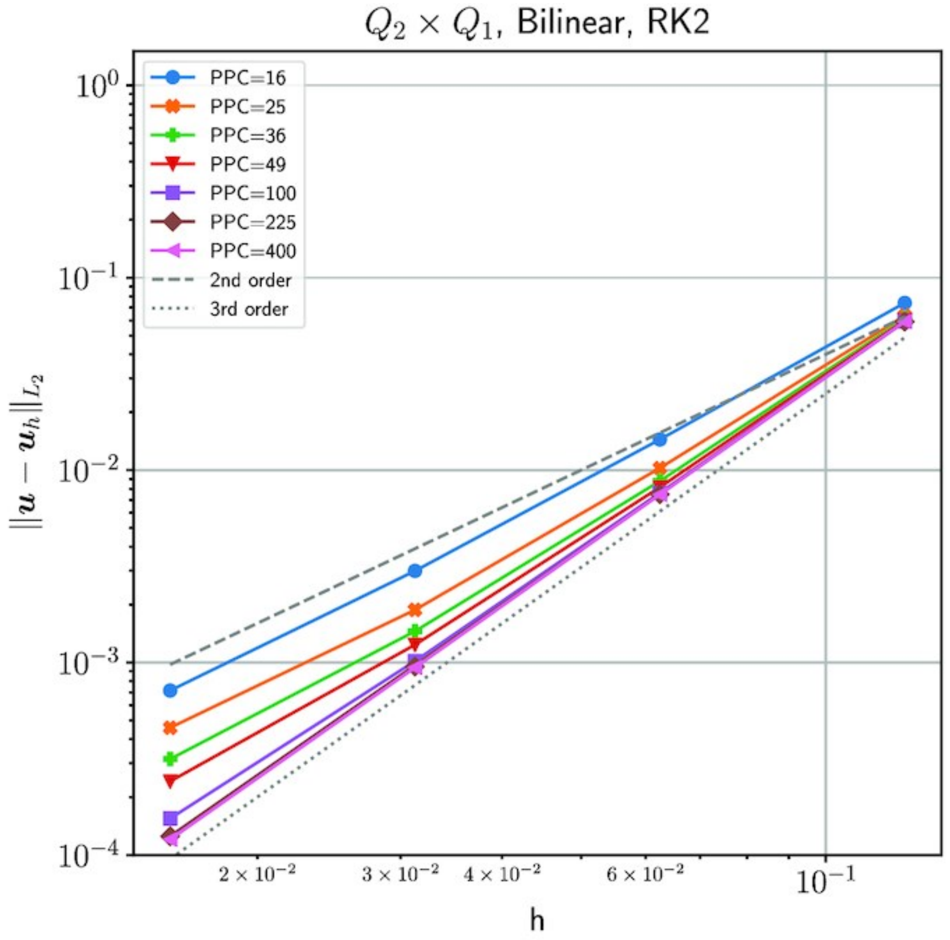
BENCHMARKING ASPECT – STOKES SOLVER

- Start with perfect knowledge of density, only solve the Stokes equations
- The difference between numerical and analytical solution (=numerical error) should disappear for infinite resolution ($h \rightarrow 0$)
- Different numerical methods produce varying error magnitudes and convergence rates (= they are differently accurate)
- All of ASPECT's finite element choices converge according to mathematical theory (Gassmöller et al., 2019)



BENCHMARKING ASPECT – PARTICLE INTERPOLATION

- Interpolation of particle property to fields can control accuracy of Stokes solution
- Linear least squares interpolation requires increasingly many particles per cell (PPC) (Gassmoeller et al., 2019).
- Quadratic least squares reaches optimal convergence with small and constant PPC (Gregory et al., in prep)



$Q_2 \times Q_1$

$\|\boldsymbol{u} - \boldsymbol{u}_h\|_{L_2}$	Direct Method		AA (16 PPC)		LLS (1024 PPC)		QLS (16 PPC)	
h	error	rate	error	rate	error	rate	error	rate
$\frac{1}{8}$	$1.07 \cdot 10^{-06}$		$6.44 \cdot 10^{-06}$		$1.71 \cdot 10^{-06}$		$1.09 \cdot 10^{-06}$	
$\frac{1}{16}$	$2.33 \cdot 10^{-07}$	2.20	$1.53 \cdot 10^{-06}$	2.07	$2.47 \cdot 10^{-07}$	2.79	$2.34 \cdot 10^{-07}$	2.23
$\frac{1}{32}$	$3.45 \cdot 10^{-08}$	2.76	$3.80 \cdot 10^{-07}$	2.01	$3.50 \cdot 10^{-08}$	2.82	$3.45 \cdot 10^{-08}$	2.76
$\frac{1}{64}$	$4.50 \cdot 10^{-09}$	2.94	$9.49 \cdot 10^{-08}$	2.00	$4.52 \cdot 10^{-09}$	2.95	$4.50 \cdot 10^{-09}$	2.94
$\frac{1}{128}$	$5.68 \cdot 10^{-10}$	2.98	$2.37 \cdot 10^{-08}$	2.00	$5.69 \cdot 10^{-10}$	2.99	$5.68 \cdot 10^{-10}$	2.99
$\frac{1}{256}$	$7.12 \cdot 10^{-11}$	3.00	$5.91 \cdot 10^{-09}$	2.00	$7.14 \cdot 10^{-11}$	3.00	$7.12 \cdot 10^{-11}$	3.00
$\frac{1}{512}$	$8.91 \cdot 10^{-12}$	3.00	$1.48 \cdot 10^{-09}$	2.00	$8.98 \cdot 10^{-12}$	2.99	$8.91 \cdot 10^{-12}$	3.00
$\frac{1}{1024}$	$1.11 \cdot 10^{-12}$	3.00	$3.69 \cdot 10^{-10}$	2.00	$1.15 \cdot 10^{-12}$	2.97	$1.11 \cdot 10^{-12}$	3.00

BENCHMARKING ASPECT – PARTICLE ADVECTION

- Advecting particles is one of the major sources of error in particle algorithms
- A sum of multiple error sources:

$$\frac{d}{dt}\tilde{\mathbf{x}}_k(t) = \tilde{\mathbf{u}}_h(\mathbf{x}_k(t), t)$$

$$\begin{aligned} \|\mathbf{x}_k(T) - \tilde{\mathbf{x}}_{k,h}(T)\| \leq\ & C_1(T)\Delta t_{\mathrm{p}}^q \\ & + C_2(T)\|\mathbf{u} - \mathbf{u}_h\| \\ & + C_3(T)\|\mathbf{u}_h - \tilde{\mathbf{u}}_h\| \end{aligned}$$

- Spatial and temporal error may behave differently, e.g.:

$$\mathbf{k}_1 = \frac{\Delta t}{2}\tilde{\mathbf{u}}_h(t^n, \mathbf{x}^n),$$

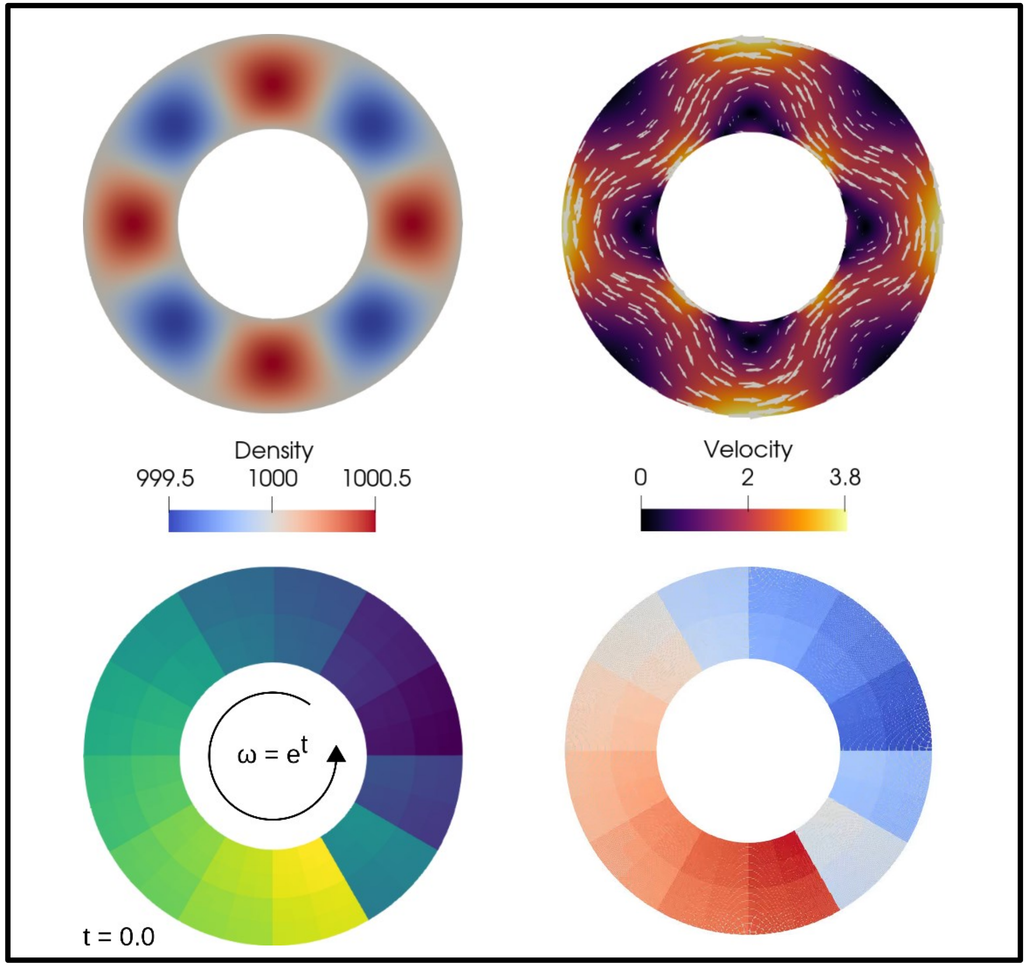
RK2: $$\mathbf{x}^{n+1} = \mathbf{x}^n + \Delta t\ \tilde{\mathbf{u}}_h\left(t^n + \frac{\Delta t}{2}, \mathbf{x}^n + \frac{\mathbf{k}_1}{2}\right)$$

RK2 FOT: $$\mathbf{x}^{n+1} = \mathbf{x}^n + \Delta t\ \tilde{\mathbf{u}}_h\left(t^n, \mathbf{x}^n + \frac{\mathbf{k}_1}{2}\right)$$

- Second order convergence in space, second or first order in time
- How to benchmark if this matters?
- Approach: Combine stationary solution with time-dependent lateral flow (Gassmöller et al., 2024)

BENCHMARKING ASPECT – PARTICLE ADVECTION

- Combine steady-state solution with time-dependent lateral flow



$$-\Delta \boldsymbol{u} + \nabla p = \rho \boldsymbol{g},$$
$$\nabla \cdot \boldsymbol{u} = 0.$$

Stokes equations

$$\Psi(r,\theta,t) = -(\frac{A}{2}r^2 + Bln(r) - 1)(\cos k\theta - \tau(t)),$$

$$\left.\begin{aligned} v_r(r,\theta,t) &= g(r)k\sin(k\theta - \tau(t)), \\ v_\theta(r,\theta,t) &= f(r)\cos(k(\theta - \tau(t))) + r\omega(t), \\ p(r,\theta,t) &= kh(r)\sin(k\theta - \tau(t)), \end{aligned}\right\} \text{Finite Elements}$$

$$\left.\rho(r,\theta,t) = \Psi(r,\theta,t),\right\} \text{Particles}$$

$$g_r(r,\theta,t) = \aleph(r)k\sin(k\theta - \tau(t))/\rho(r,\theta,t),$$

$$g_\theta = 0.$$

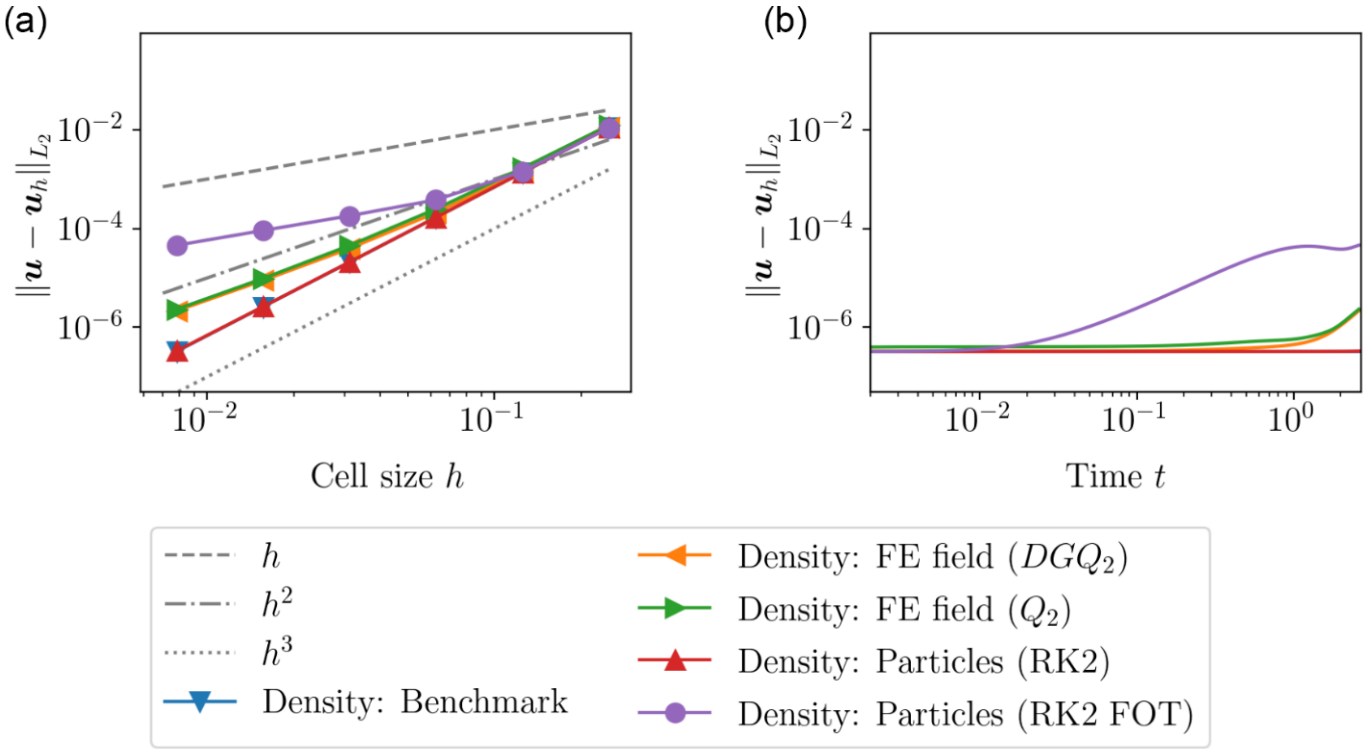
$$\tau(t) = \int_0^T \nu(t)dt.$$

(Gassmöller et al., 2024)

Benchmark available at:
https://github.com/geodynamics/aspect/tree/main/benchmarks/annulus

BENCHMARKING ASPECT – TRANSIENT FLOW

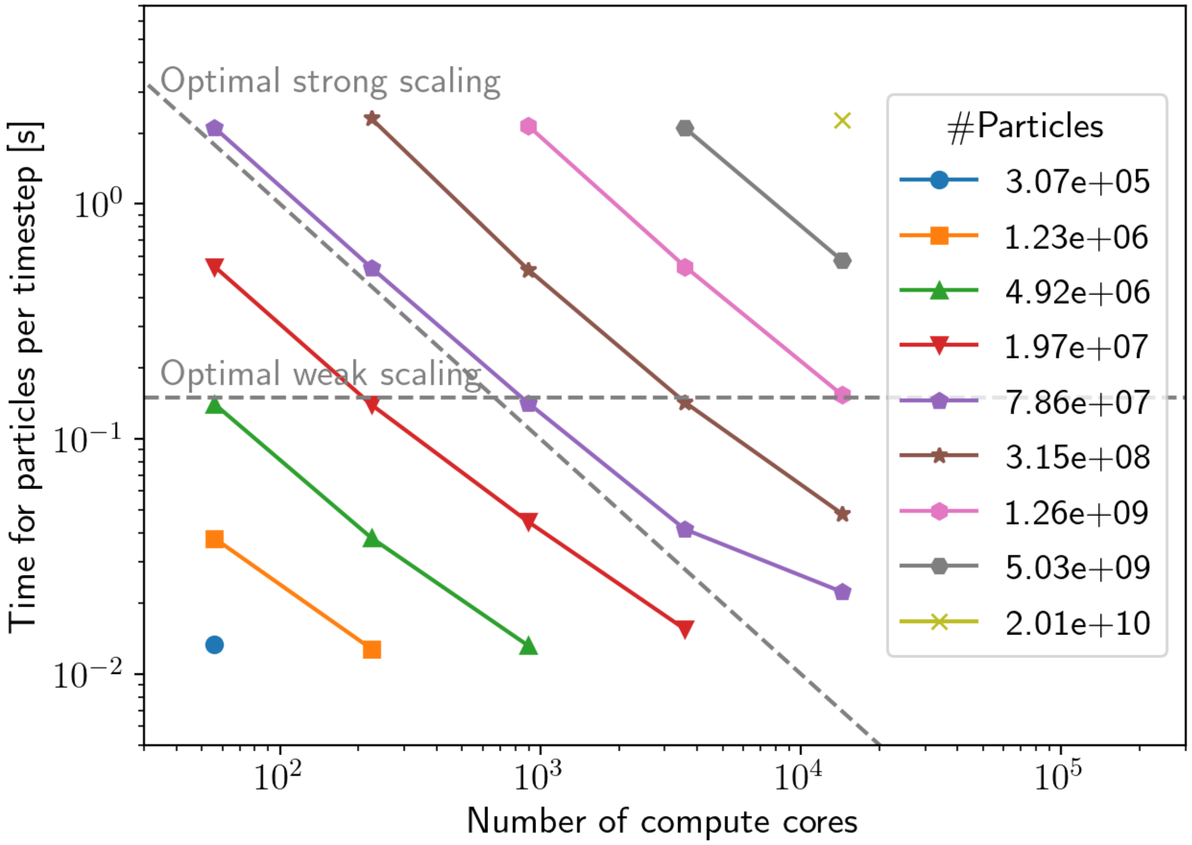
- Numerical velocity error over cell size (**h**) and time (**t**):



Benchmark available at:
https://github.com/geodynamics/aspect/tree/main/benchmarks/annulus

- Analytical density (blue) reaches third order convergence as expected
- Particles (RK2, red) reach up to third order
- Fields (orange, green) reach second order as expected
- Particles with first order time stepping (RK2 FOT, purple) only reaches first order accuracy
- Particles are not automatically better than fields

BENCHMARKING ASPECT – PERFORMANCE AND SCALABILITY



Scalability of ASPECT 2.4.0.pre, deal.II 10.0.pre, on NSF/TACC Frontera

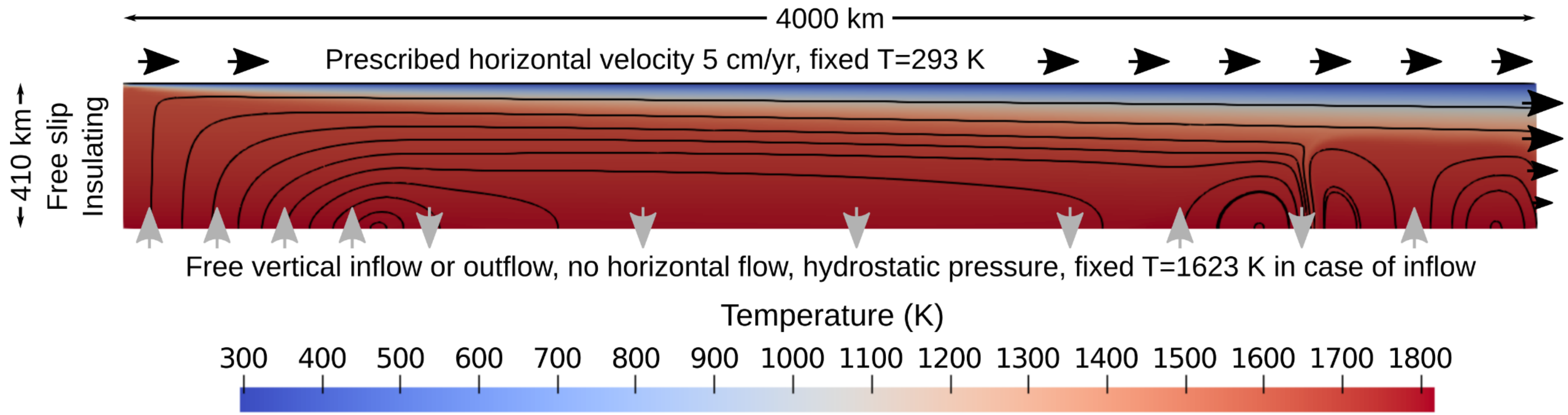
- Our implementation reaches optimal scalability from 56 to 14,336 CPU cores and ~300 thousand to 20 billion particles
- Scalability begins to taper off at <6k particles per process
- We are prepared for the next generation of HPC infrastructure

DOES ACCURACY MATTER IN PRACTICE?

LET’S CHECK AN APPLICATION

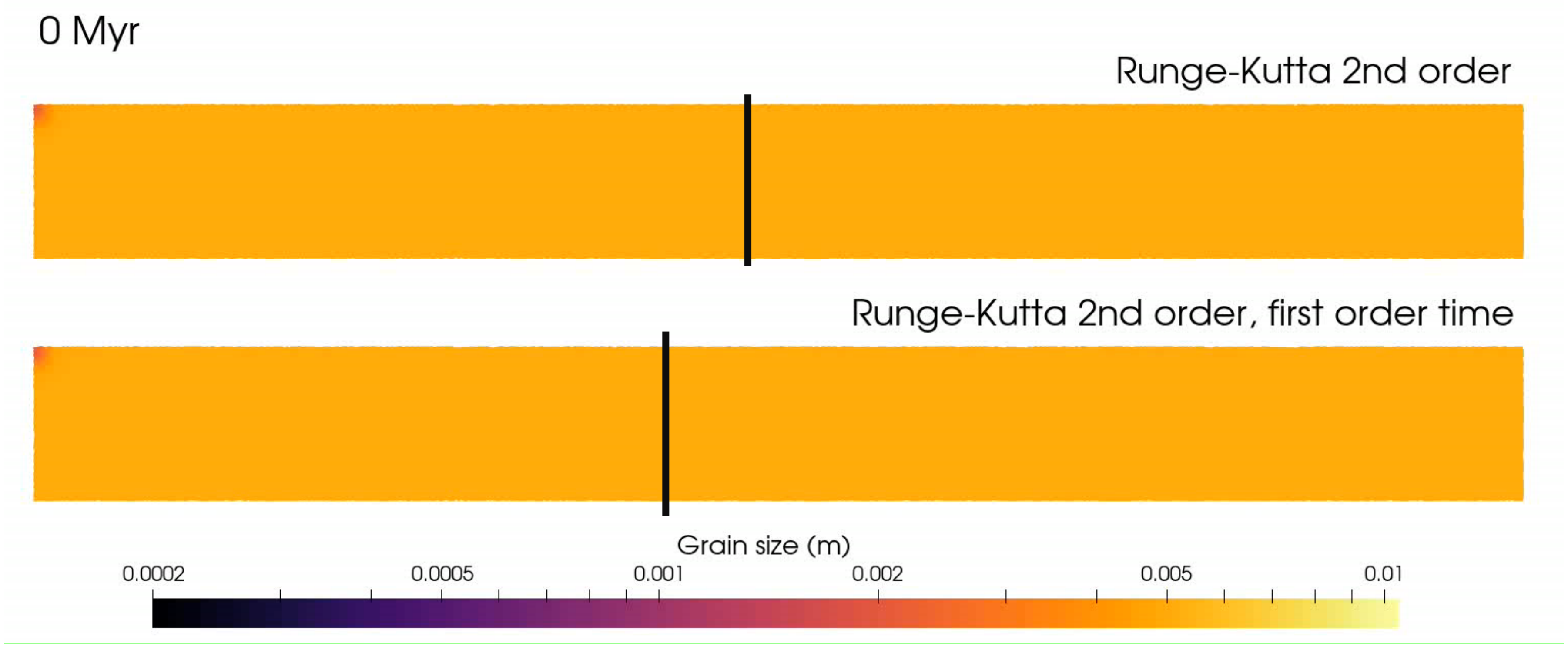
GRAIN-SIZE DEPENDENT SMALL-SCALE CONVECTION

- Model of grain-size dependent small-scale convection below an oceanic plate
- Test the difference between RK2 first order time and a true RK2 in application



DOES ACCURACY MATTER? GRAIN-SIZE DEPENDENT SMALL-SCALE CONVECTION

- Model of grain-size dependent small-scale convection below an oceanic plate
- Test the difference between RK2 first order time and a true RK2 in application
- Significant differences in time and space of onset of small-scale convection



Distance to ridge	Time of onset
1940 km	39 Myr
1710 km	34 Myr

DOES ACCURACY MATTER? GRAIN-SIZE DEPENDENT SMALL-SCALE CONVECTION

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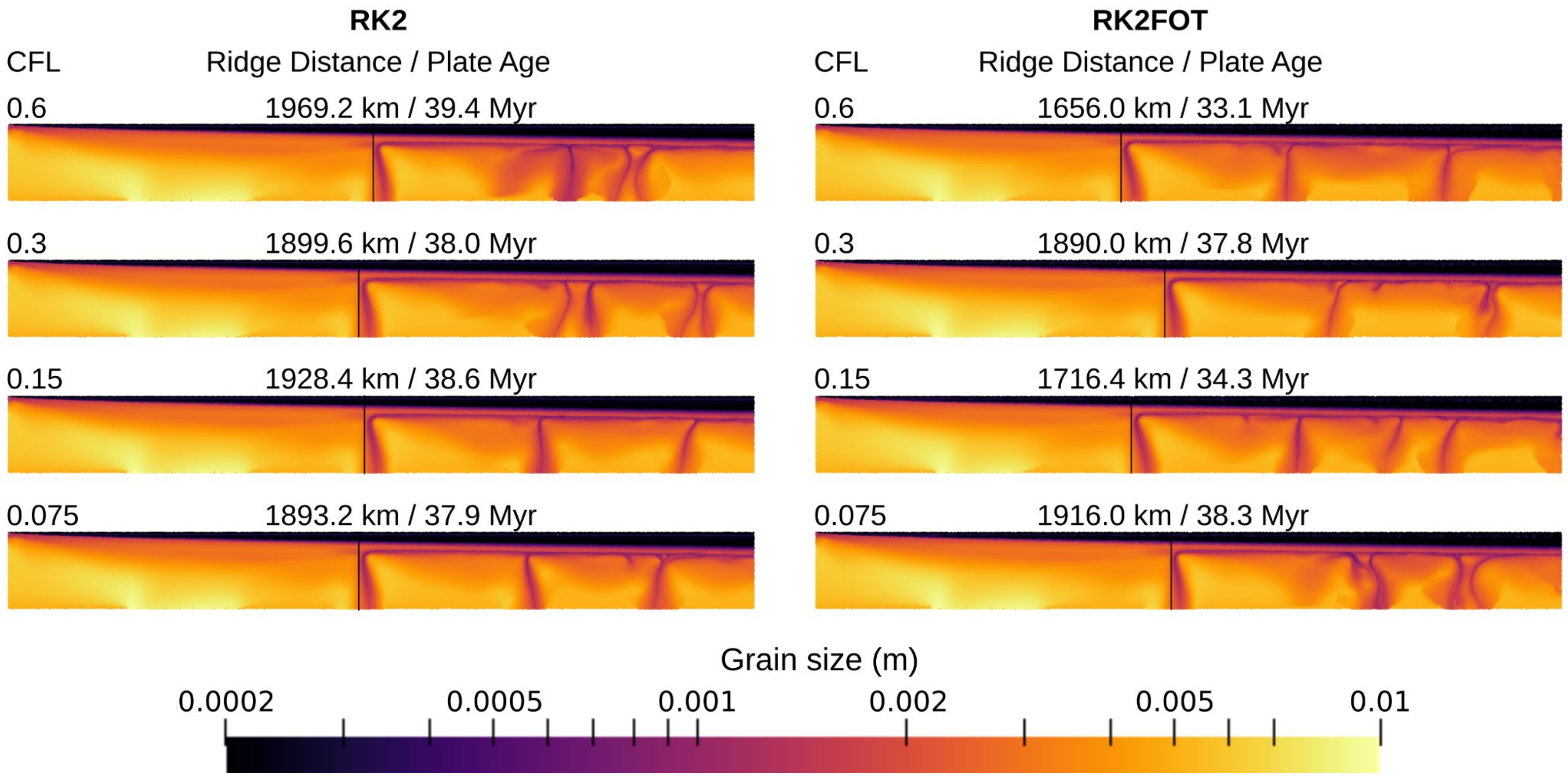
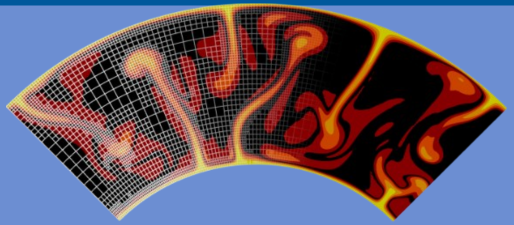
- Significant differences in time and space of onset of small-scale convection



Sub-Lithospheric Small-Scale Convection as a Window into the Asthenosphere



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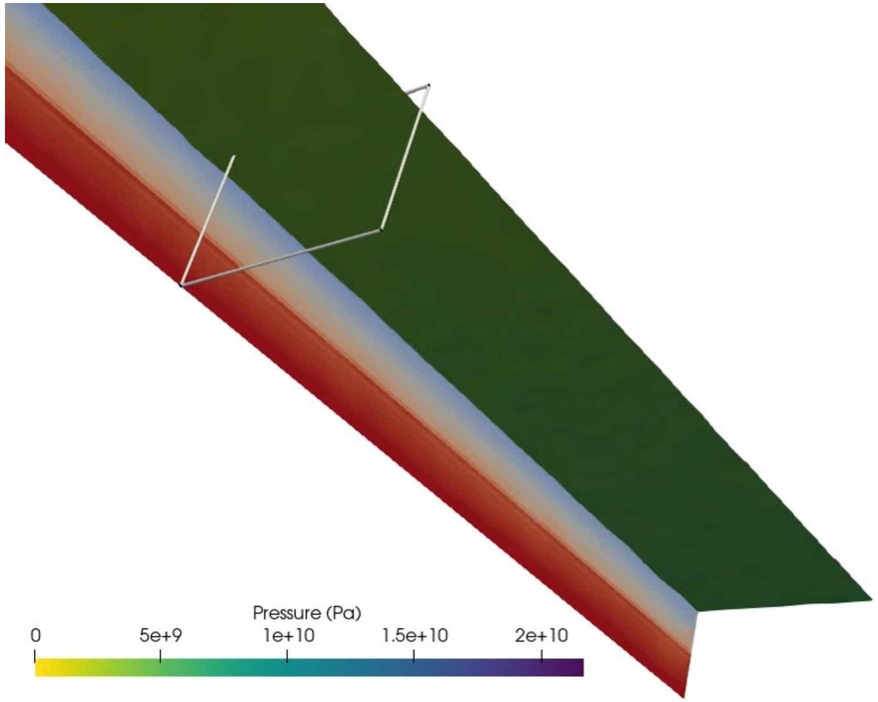

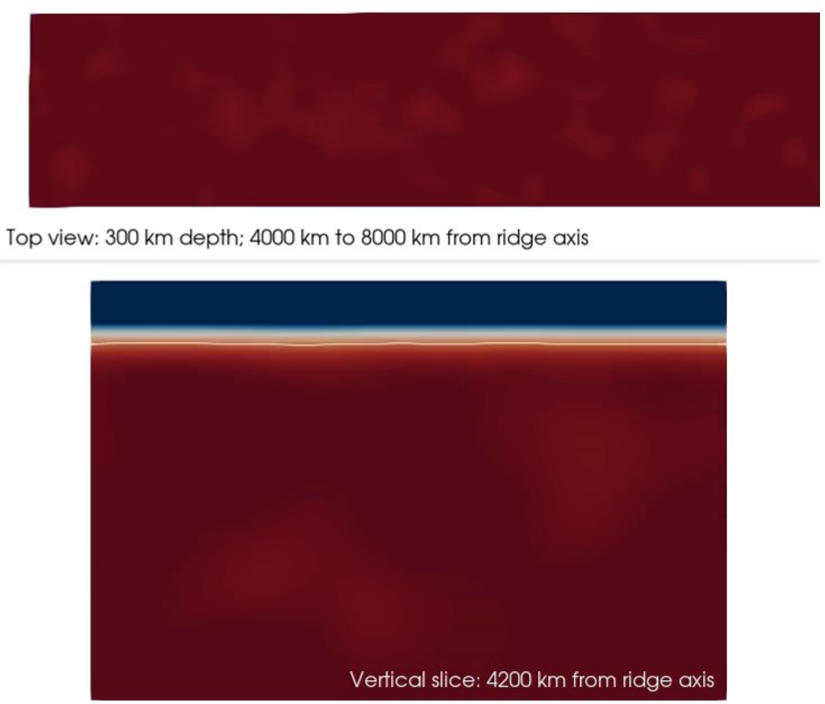

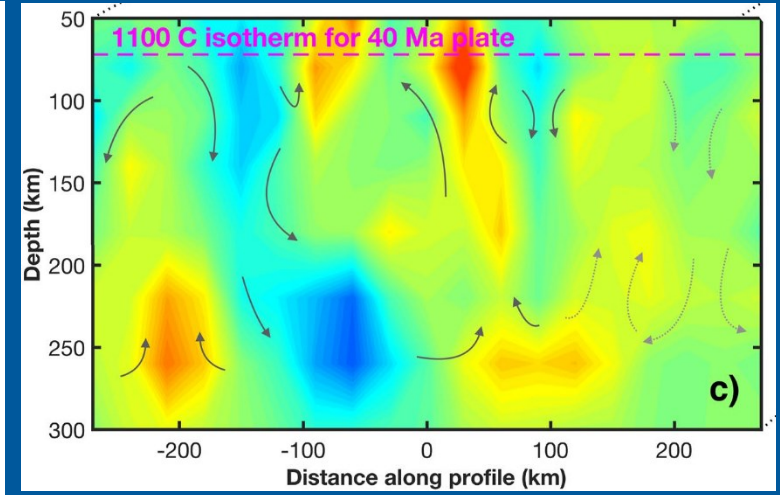

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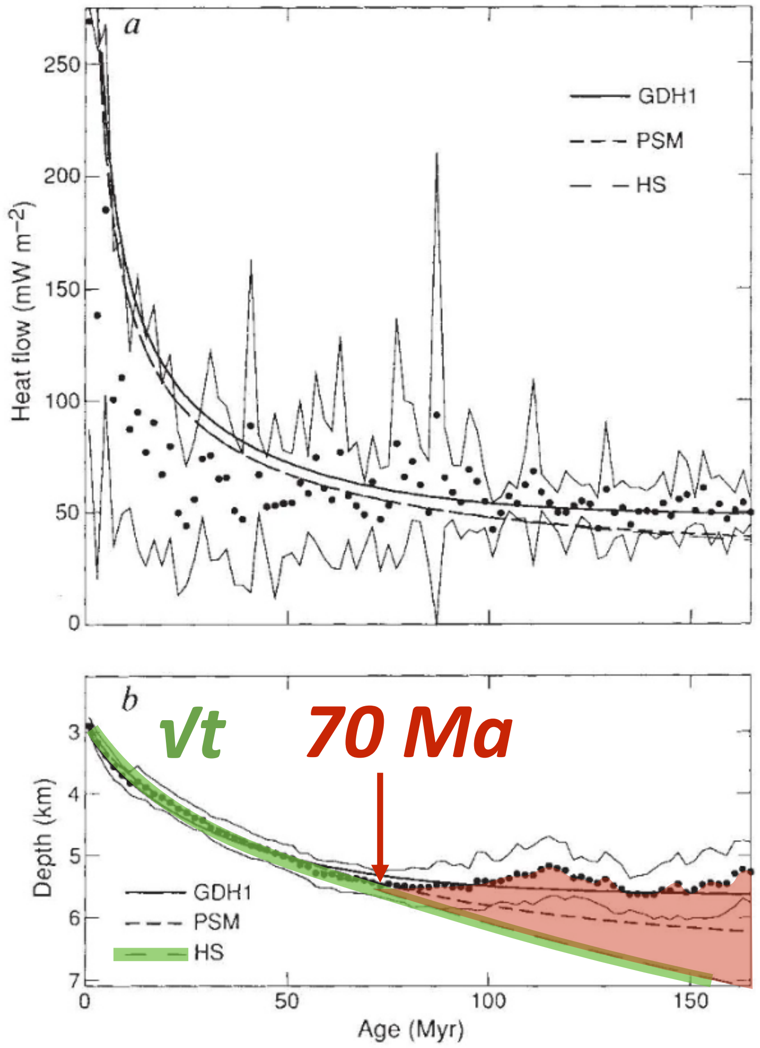
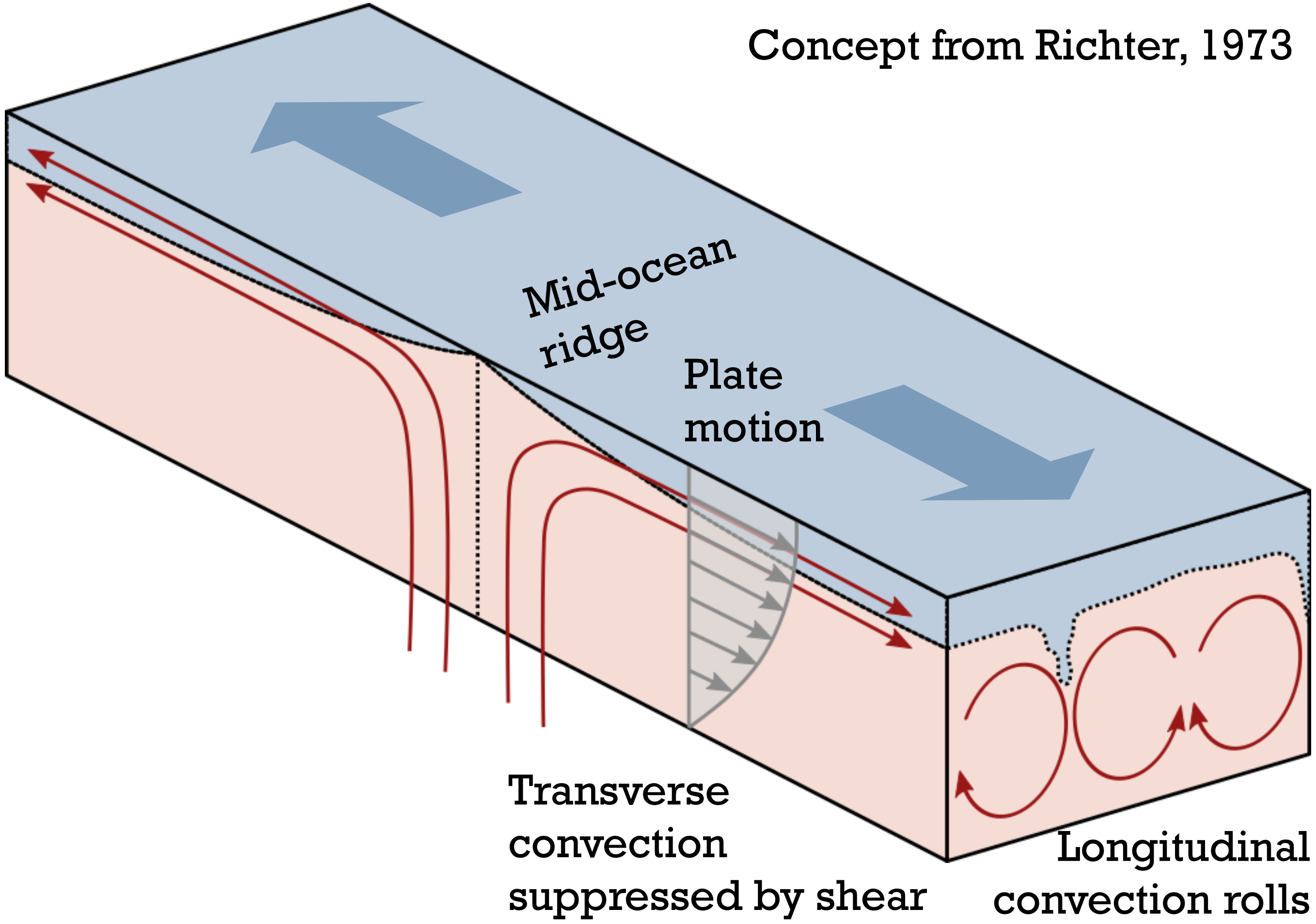
UNDERSTANDING SMALL-SCALE CONVECTION



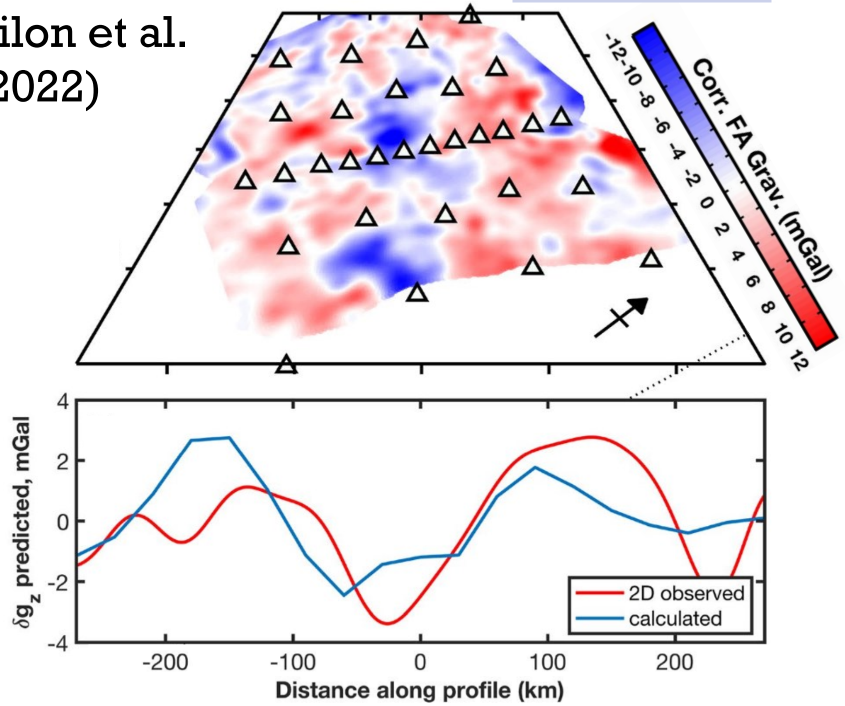
Stein & Stein, 1992

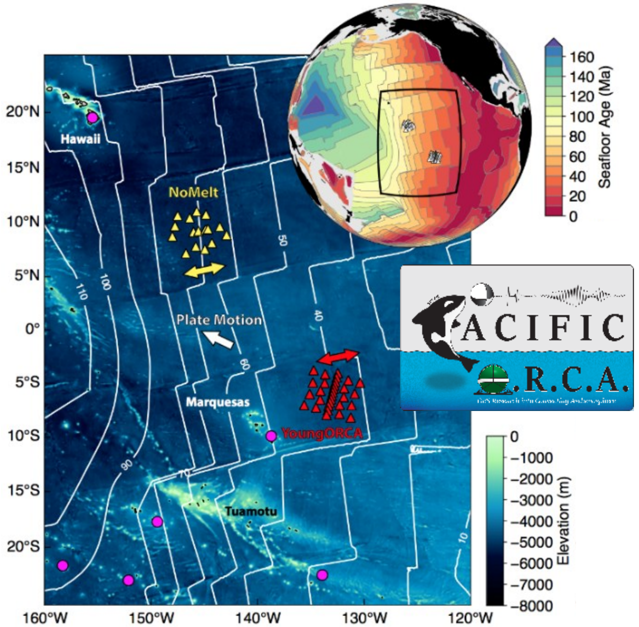


OBSERVATIONS FROM SEISMOLOGY

* 42 Ma plate age
* Lineations parallel to plate motion
* Wavelength: ~250 km

Eilon et al. (2022)

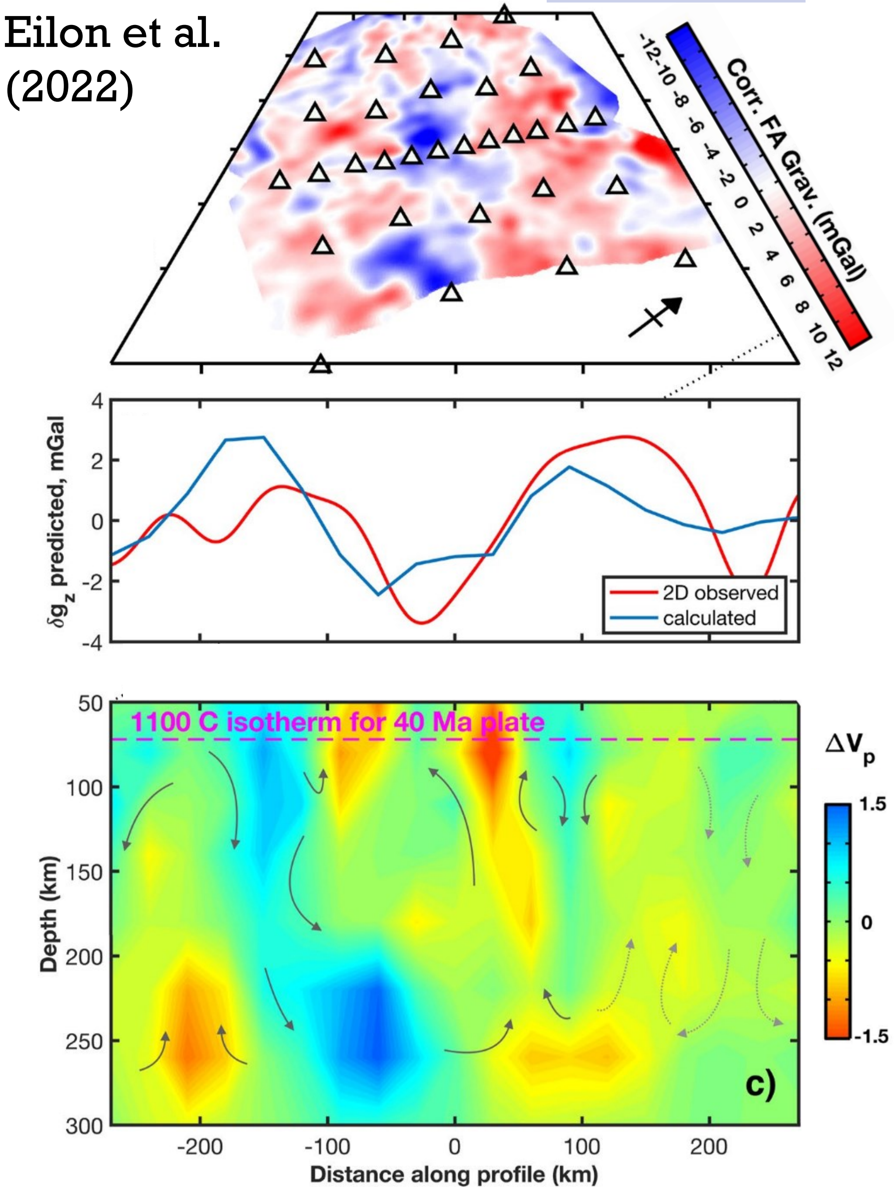


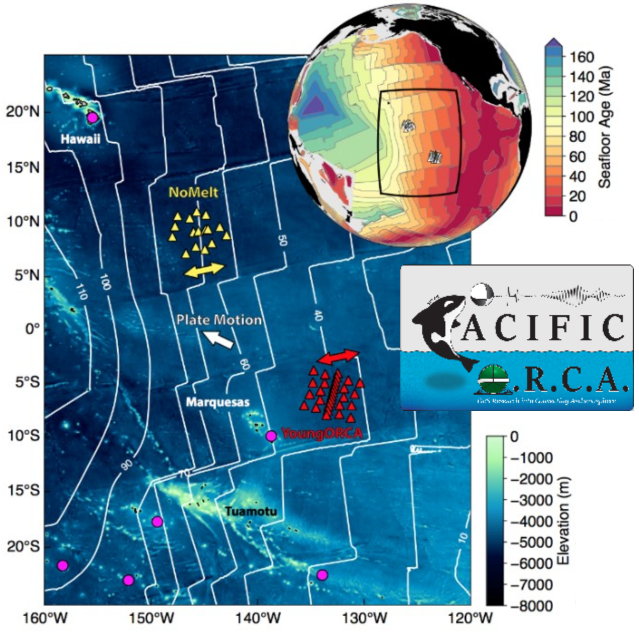


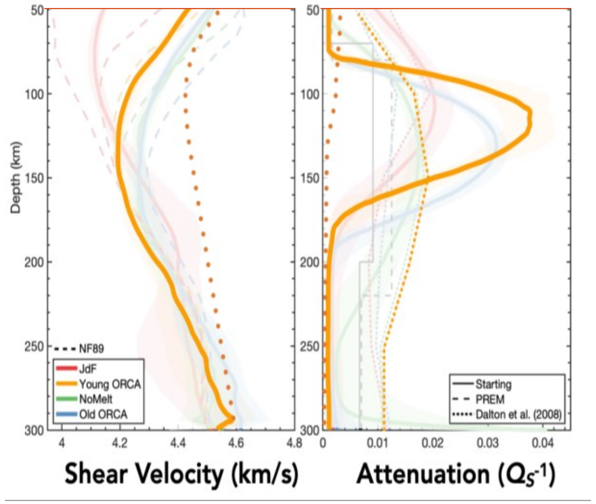
OBSERVATIONS FROM SEISMOLOGY

- Onset: 42 Ma plate age
- Lineations parallel to plate motion
- Wavelength: ~250 km
- Strongest anomalies: 180-280 km depth
- Amplitude of anomalies: ~400K if temperature alone or ~200K + 0.5% melt
- VERY high attenuation in relatively confined layer

Eilon et al. (2022)

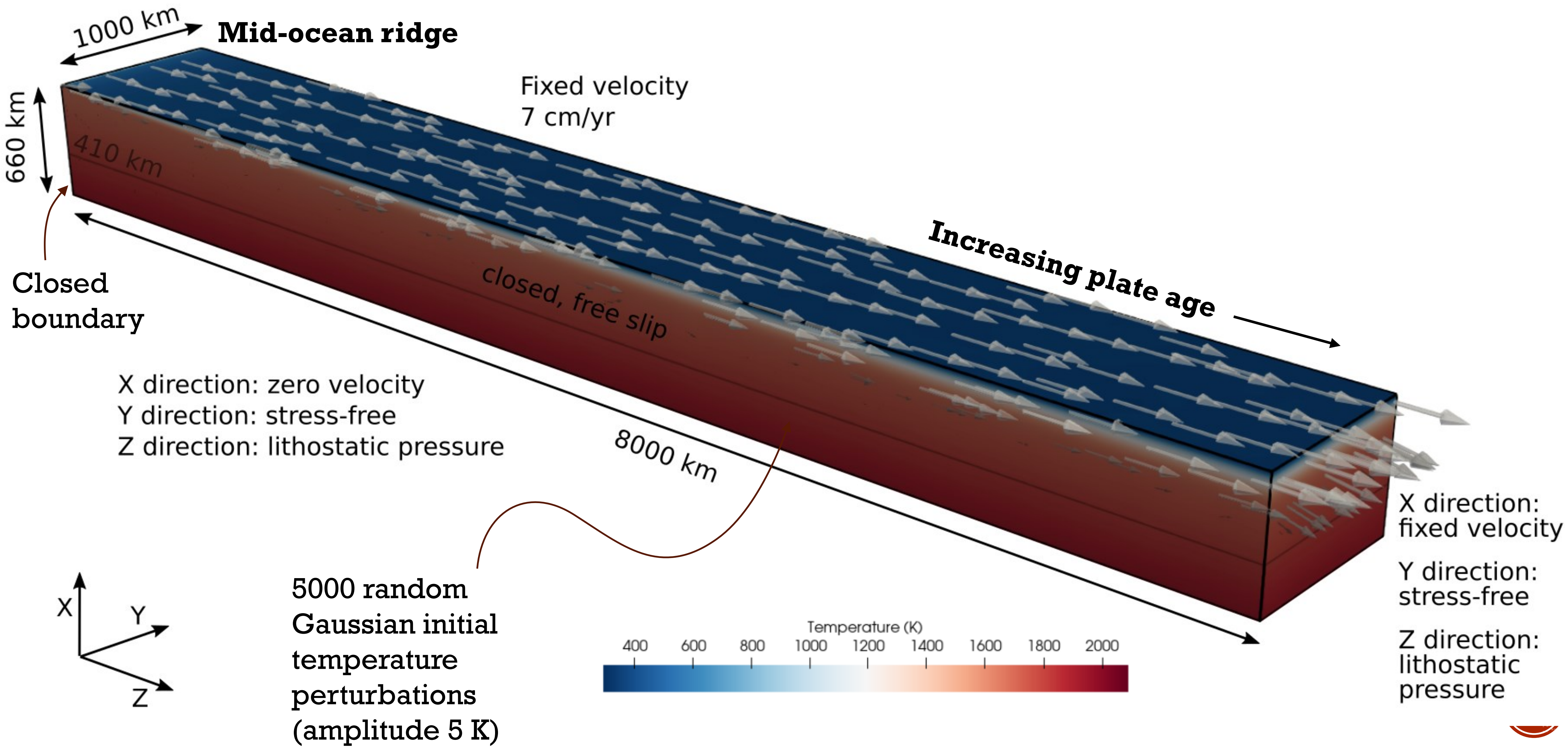






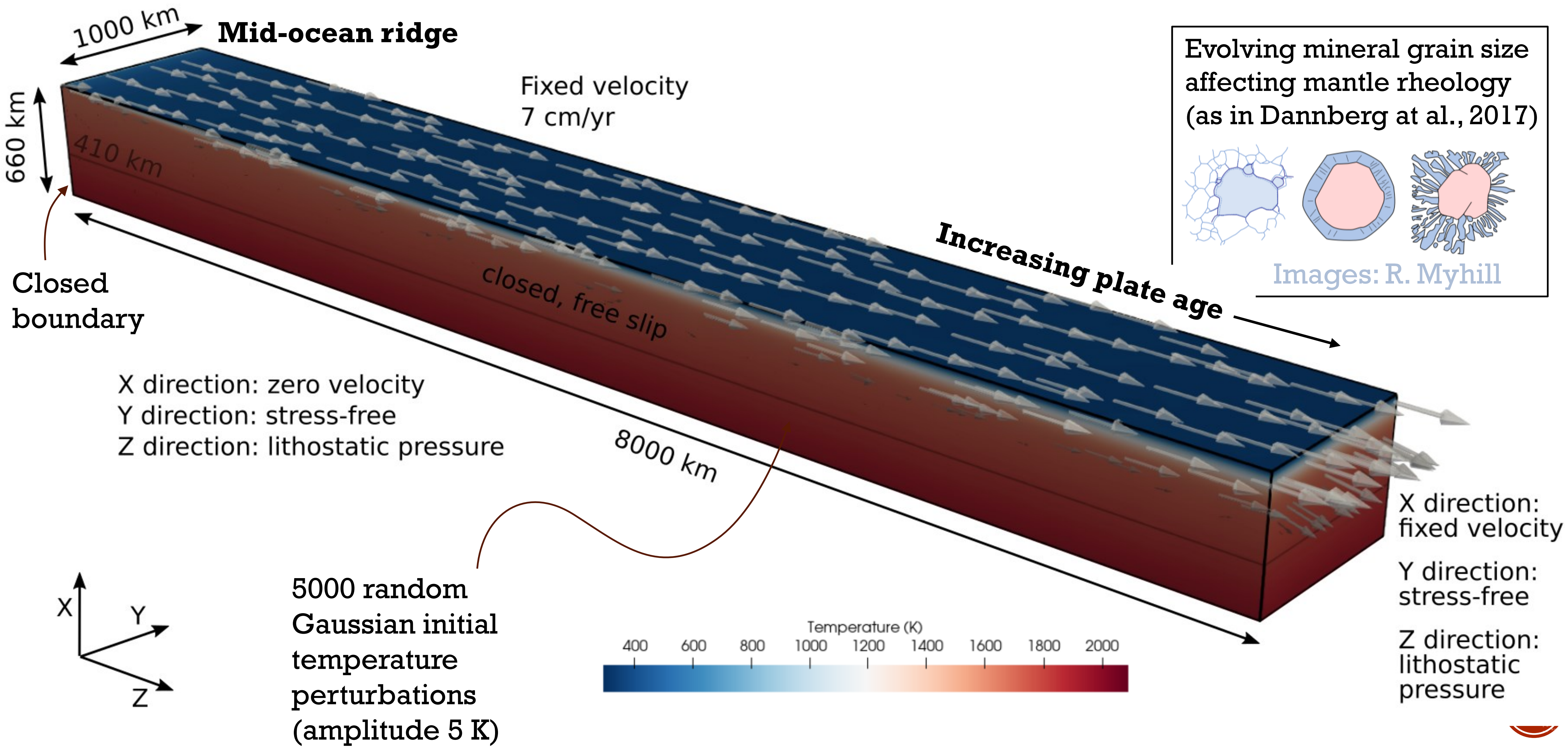
Russell et al., in prep

MODEL SETUP



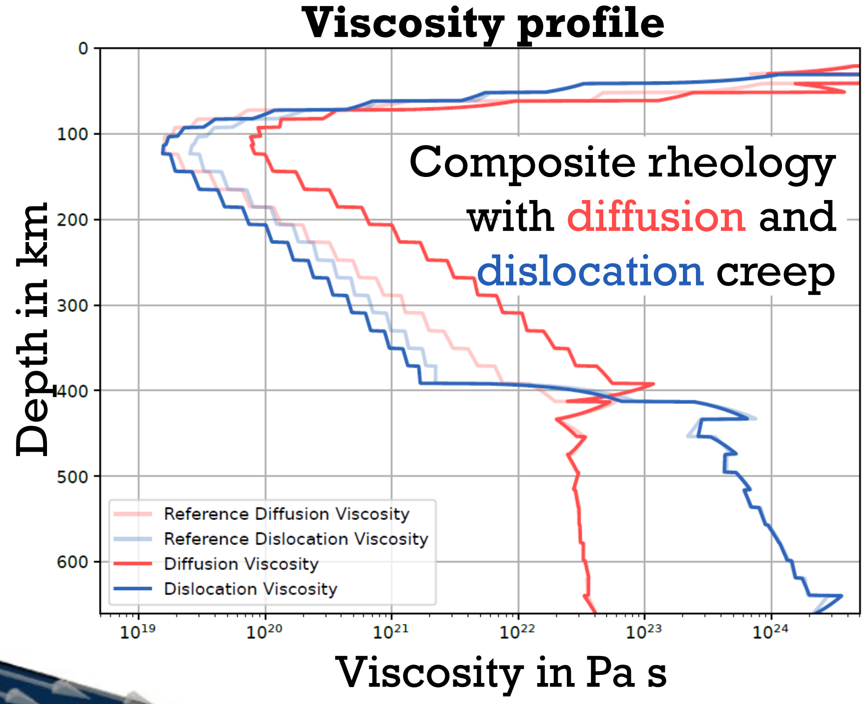
1000 km
Mid-ocean ridge
660 km
410 km
Fixed velocity
7 cm/yr
Closed
boundary
closed, free slip
Increasing plate age
X direction: zero velocity
Y direction: stress-free
Z direction: lithostatic pressure
8000 km
X direction:
fixed velocity
Y direction:
stress-free
Z direction:
lithostatic
pressure
X
Y
Z
5000 random
Gaussian initial
temperature
perturbations
(amplitude 5 K)
Temperature (K)
400
600
800
1000
1200
1400
1600
1800
2000

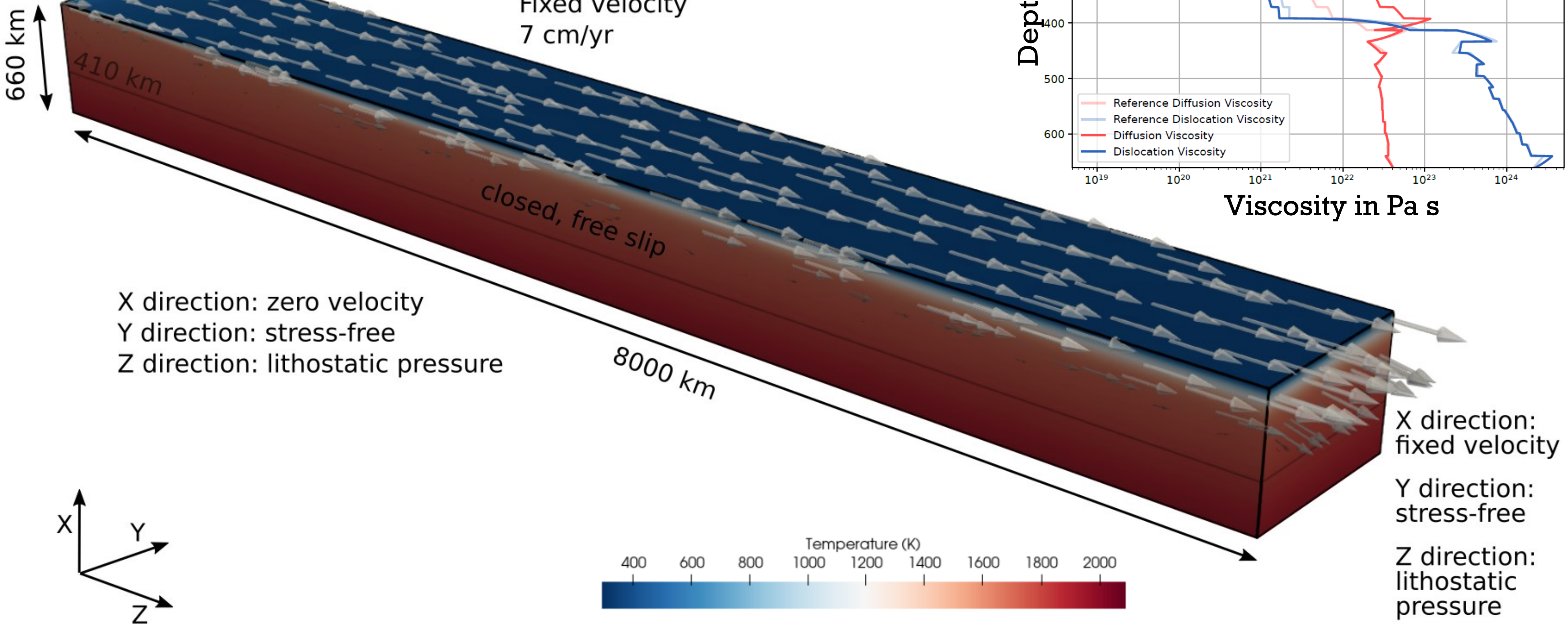
MODEL SETUP


1000 km
Mid-ocean ridge
660 km
410 km
Closed boundary
Fixed velocity
7 cm/yr
closed, free slip
Increasing plate age
8000 km
X direction: zero velocity
Y direction: stress-free
Z direction: lithostatic pressure
X direction: fixed velocity
Y direction: stress-free
Z direction: lithostatic pressure
5000 random Gaussian initial temperature perturbations (amplitude 5 K)
Temperature (K)
400 600 800 1000 1200 1400 1600 1800 2000
X
Y
Z
Evolving mineral grain size affecting mantle rheology (as in Dannberg at al., 2017)
Images: R. Myhill

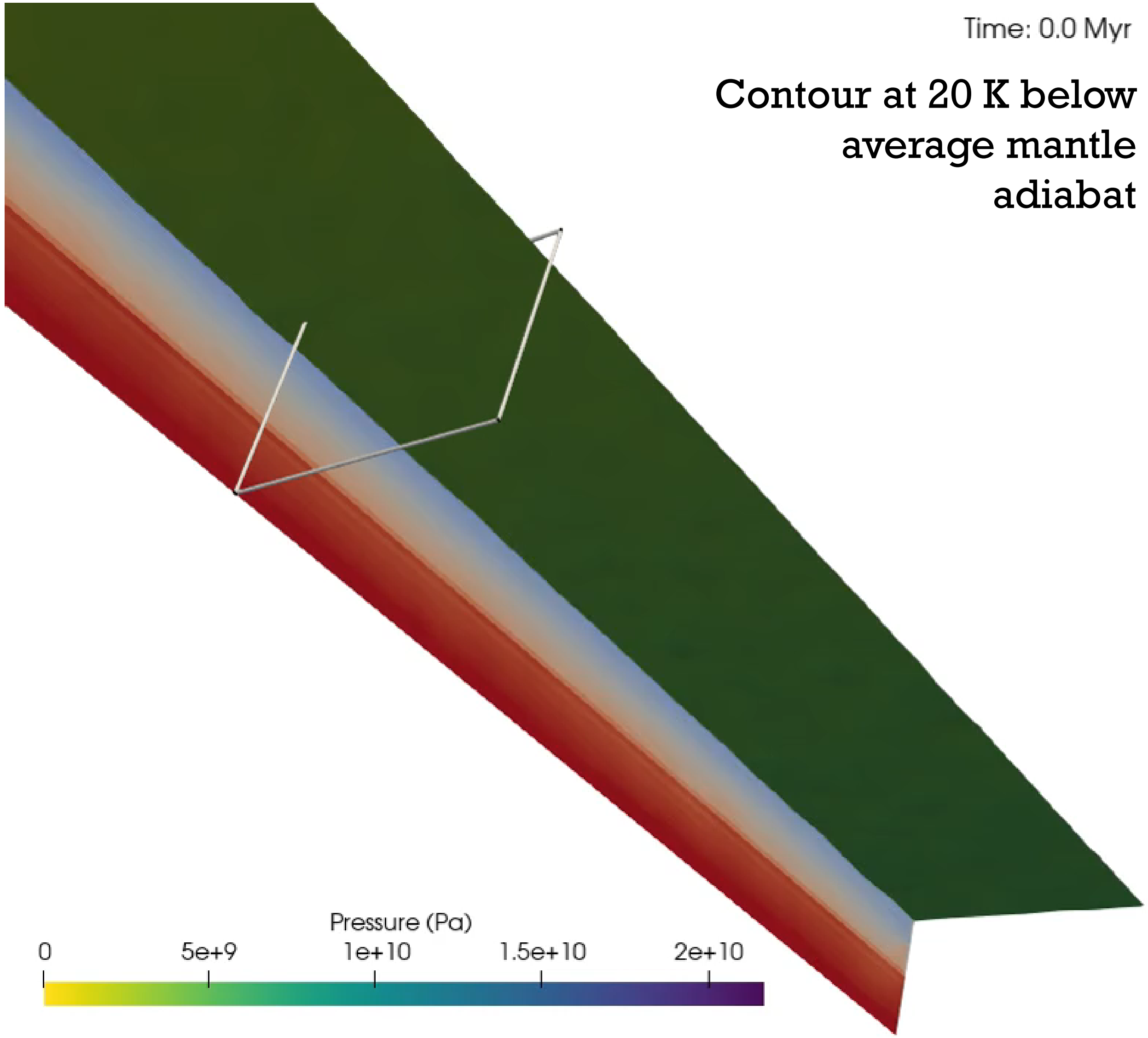
MODEL SETUP

Upper mantle rheology following Hirth and Kohlstedt [2003]

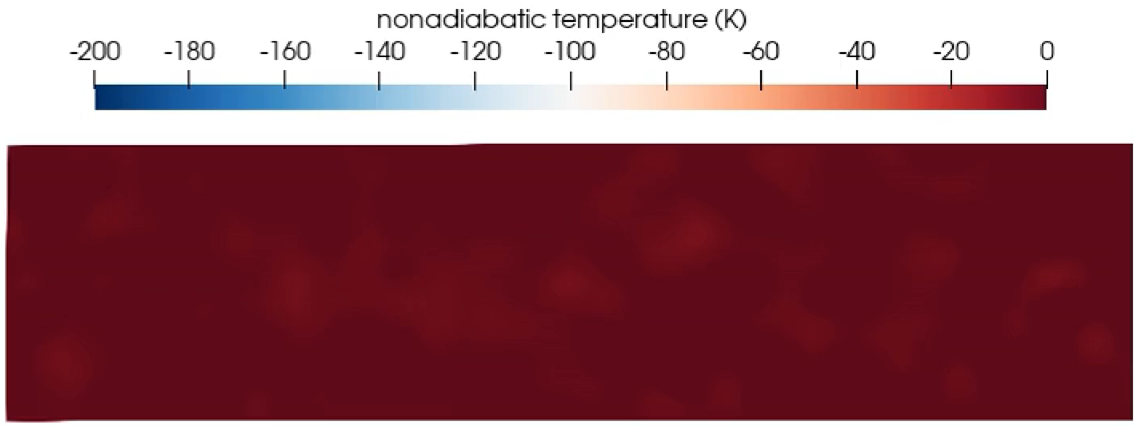




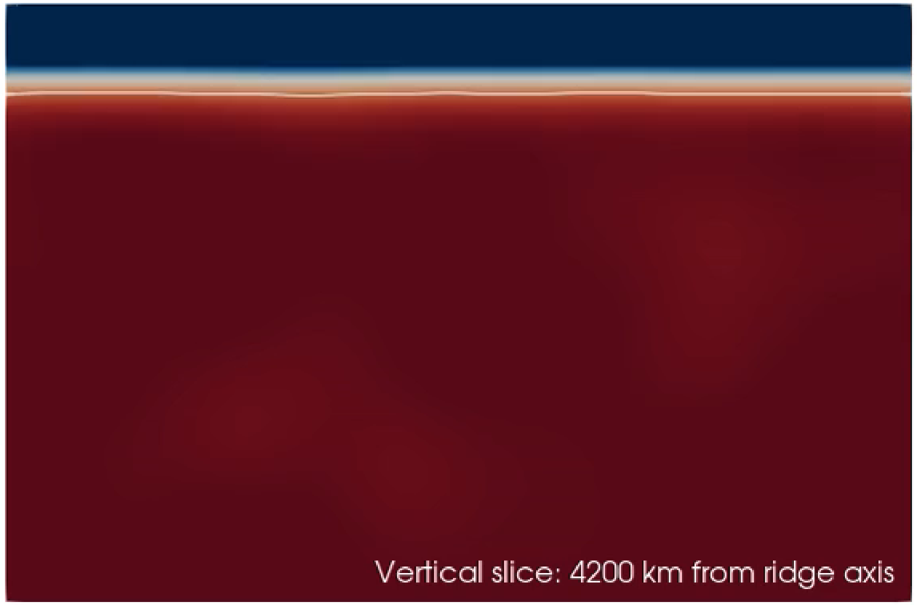
MODEL EVOLUTION



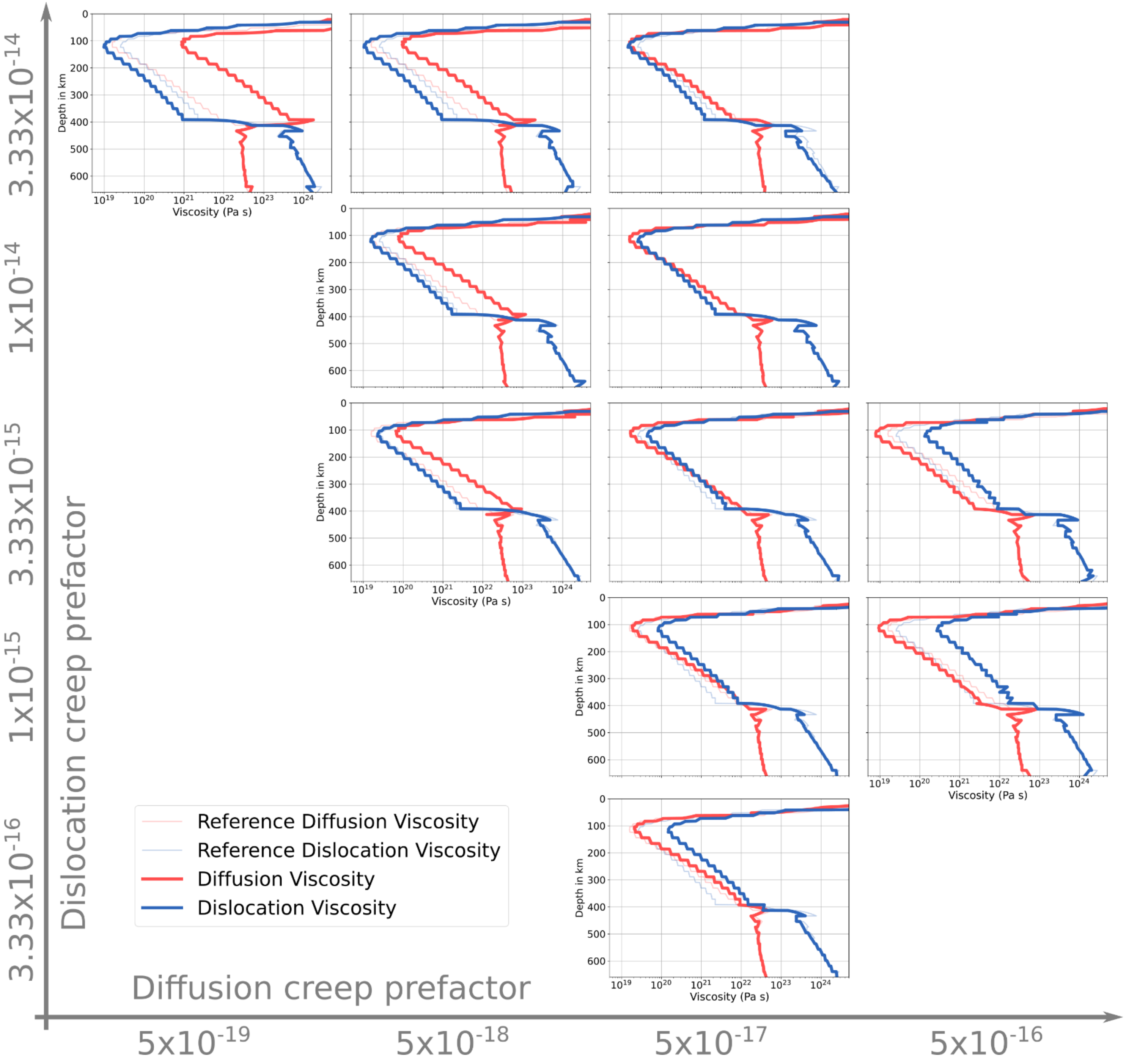
Contour at 20 K below average mantle adiabat



Top view: 300 km depth; 4000 km to 8000 km from ridge axis

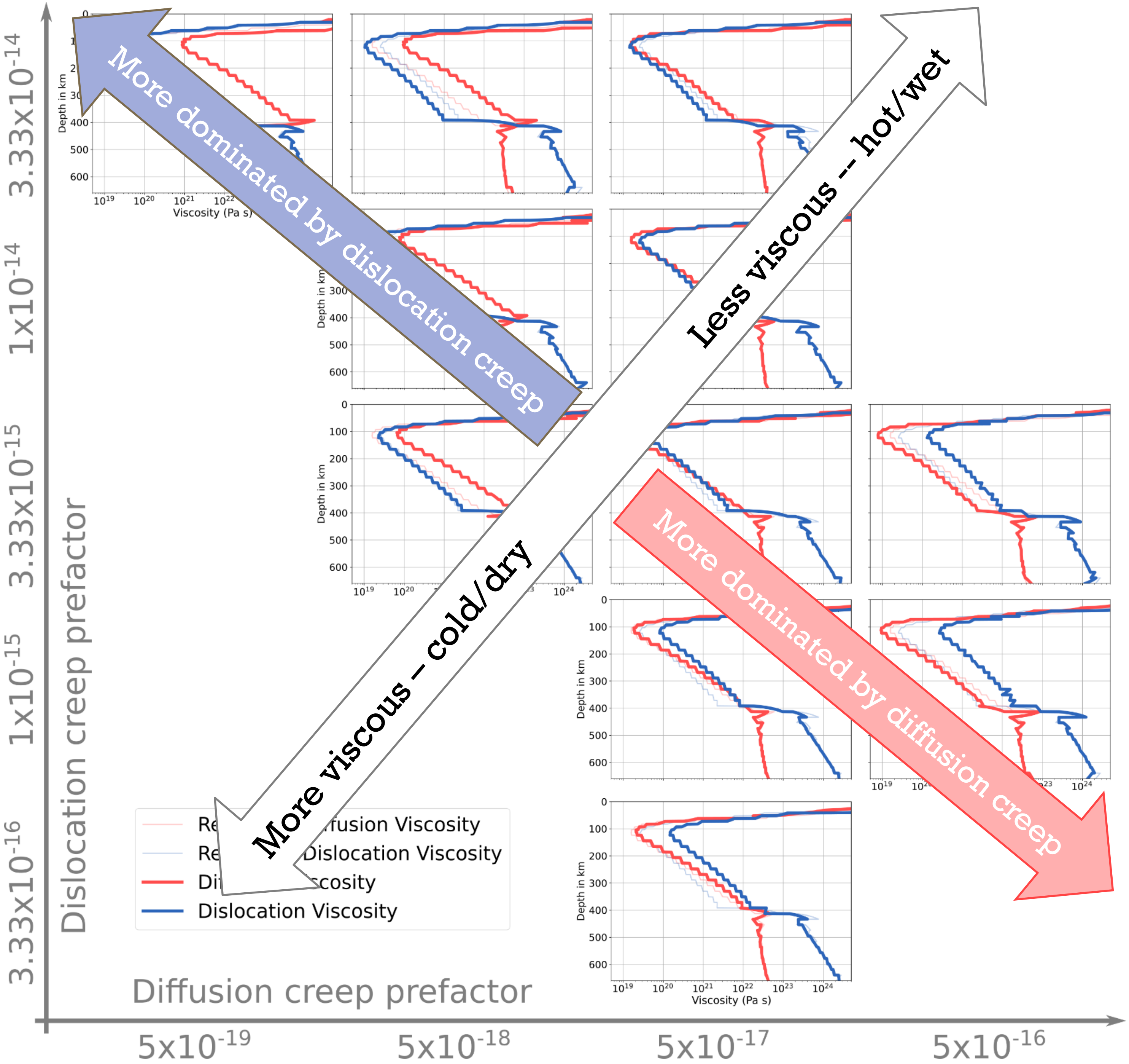


MODEL PARAMETERS



- Pre-factors of the viscous creep laws have largest uncertainties
- Changing the prefactors changes the balance between diffusion and dislocation creep and the absolute viscosity values

MODEL PARAMETERS



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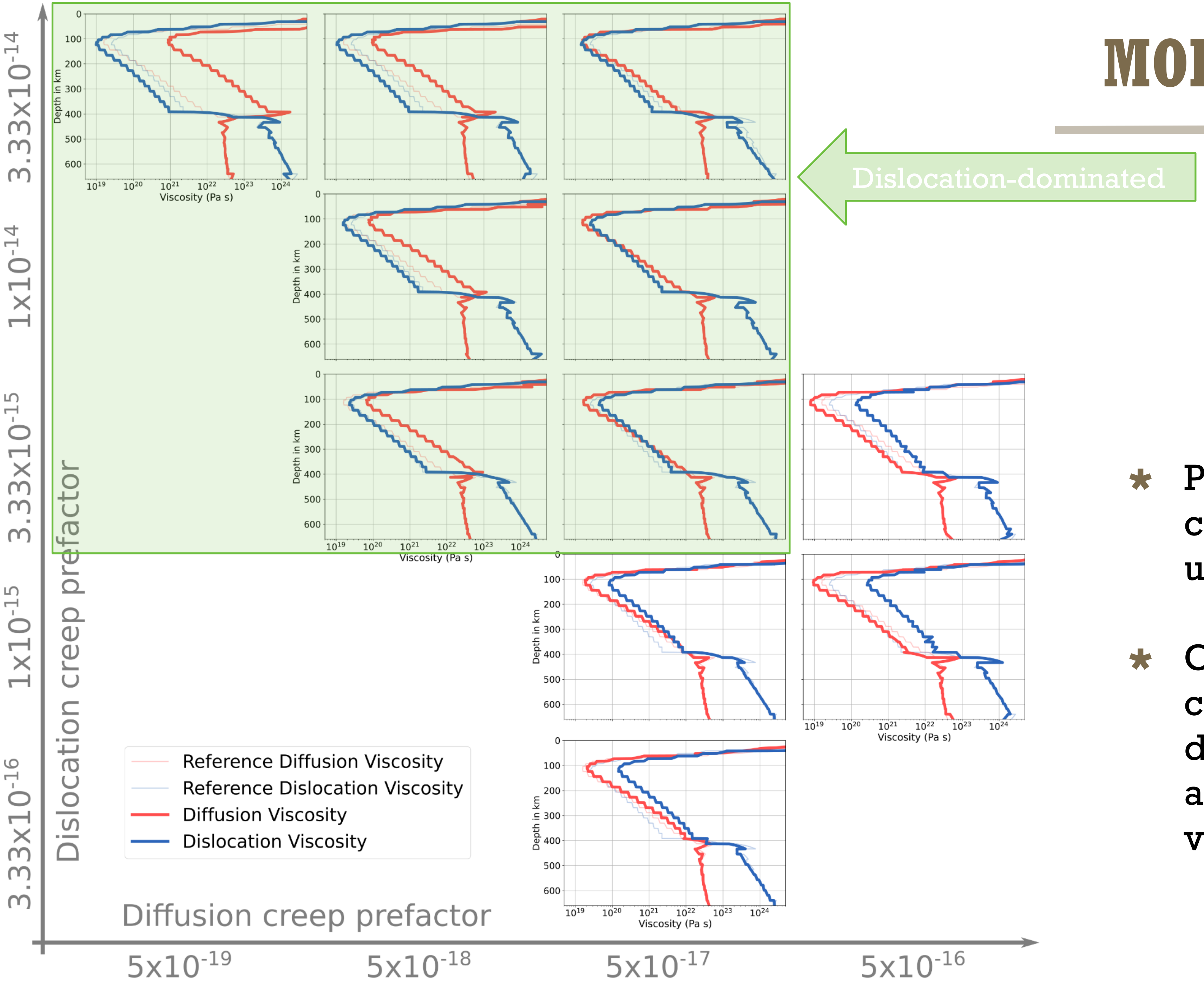
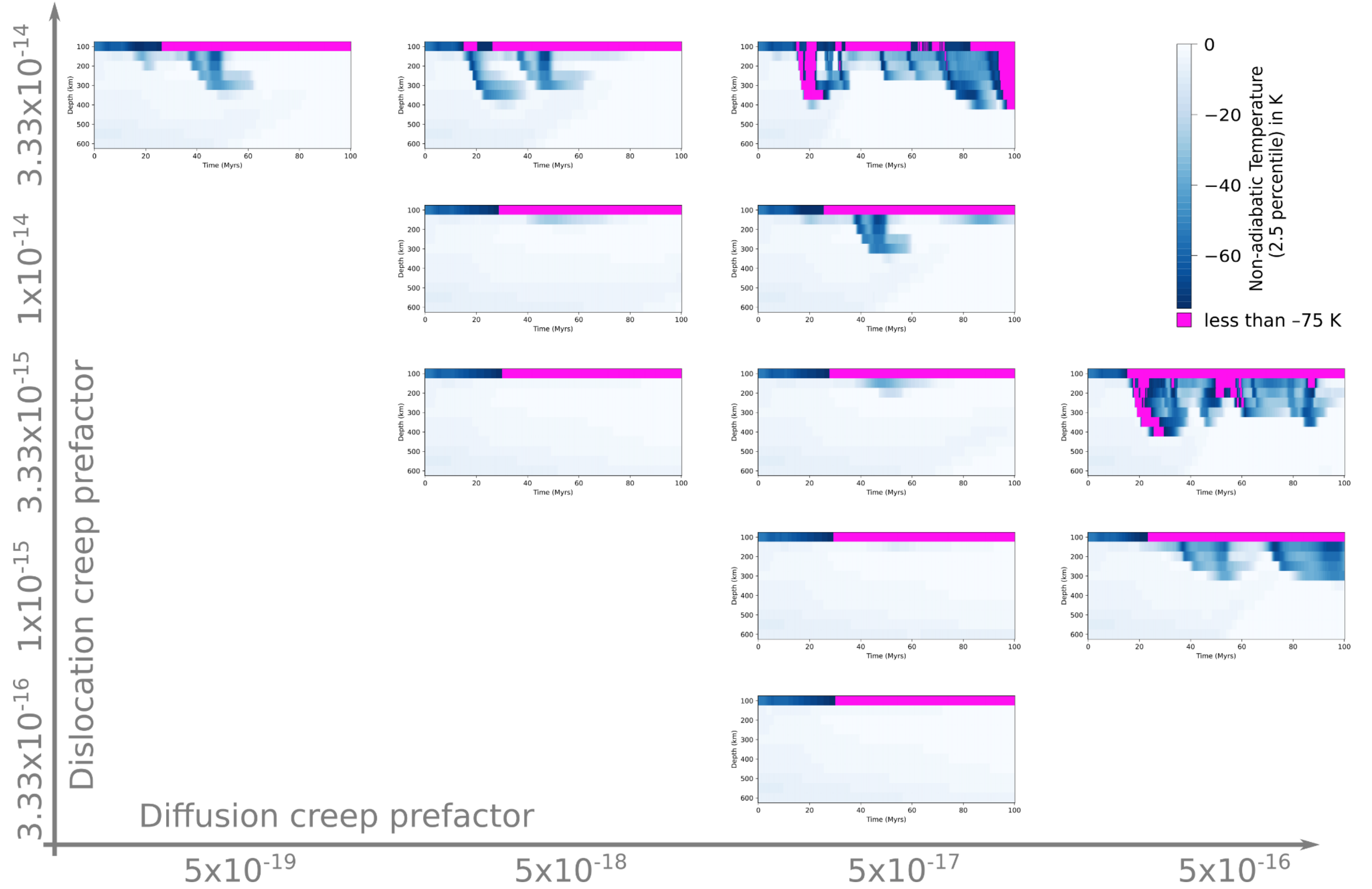
MODEL PARAMETERS



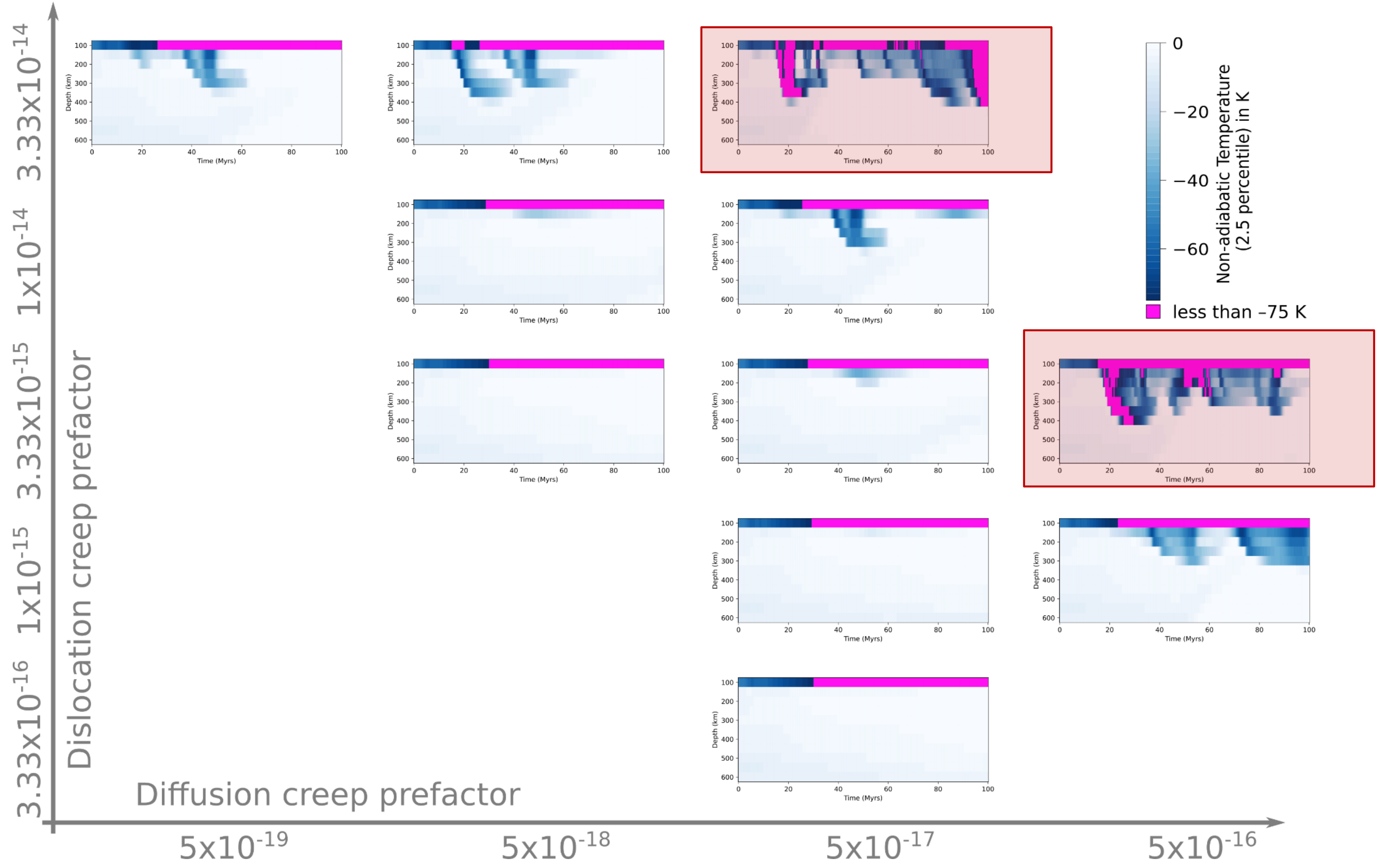
* Pre-factors of the viscous creep laws have largest uncertainties
* Changing the prefactors changes the balance between diffusion and dislocation creep and the absolute viscosity values

AMPLITUDE/DEPTH OF TEMPERATURE ANOMALIES



<-- Vertical slice through the models at 42 Ma plate age, plotted over model evolution time

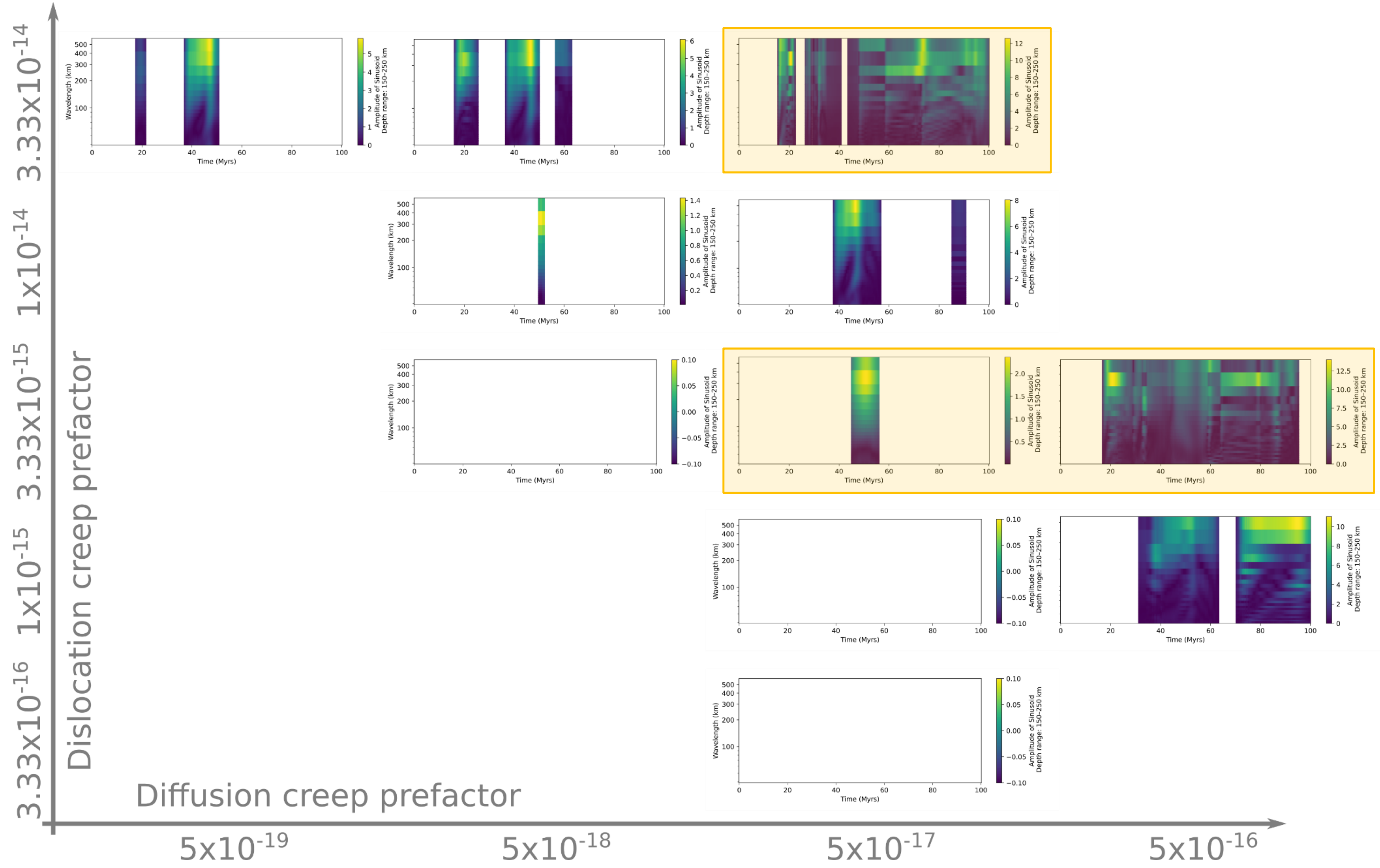
AMPLITUDE/DEPTH OF TEMPERATURE ANOMALIES



<-- Vertical slice through the models at 42 Ma plate age, plotted over model evolution time

* Only two models have anomalies that are strong enough

WAVELENGTH OF TEMPERATURE ANOMALIES

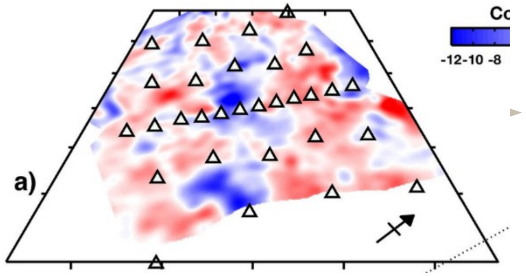


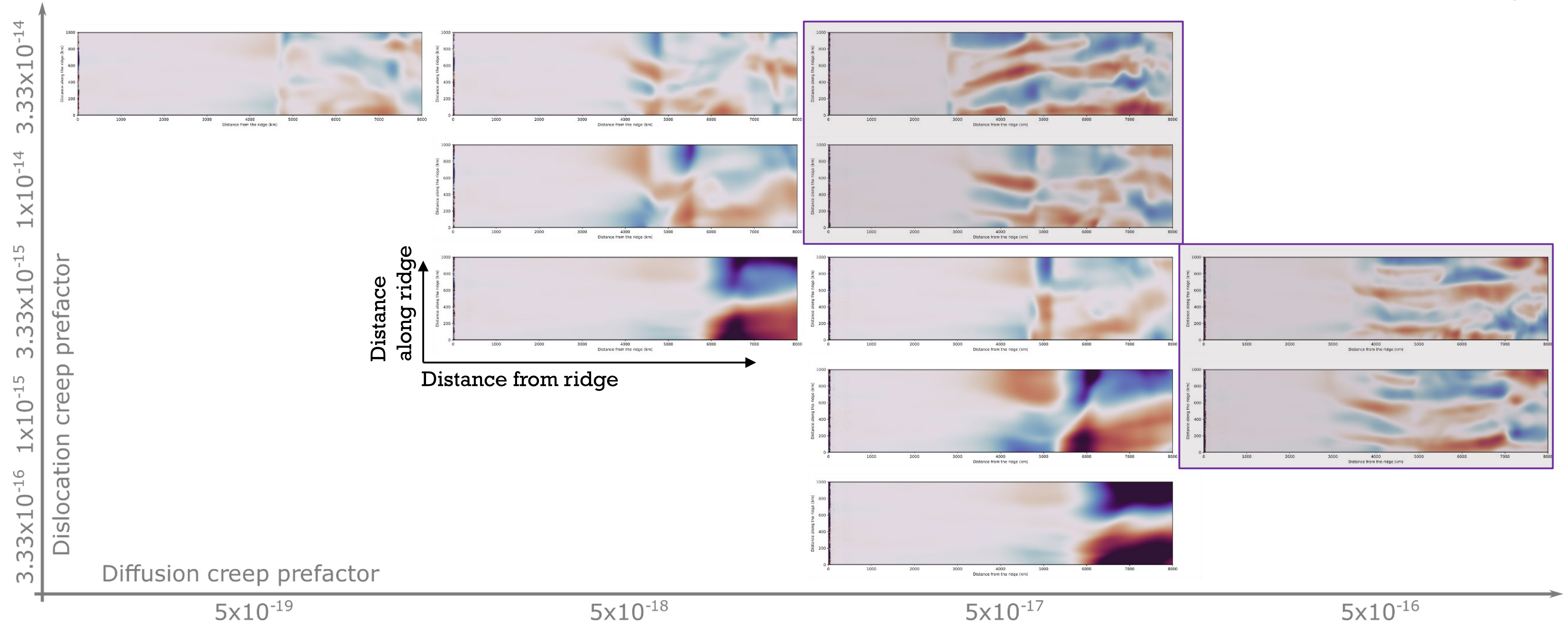
<-- Spectrum of the models at 42 Ma plate age, plotted over model evolution time

- Range of scales (150-500 km)
- low wavelength (350-500 km) dominant in many models

SURFACE EXPRESSION

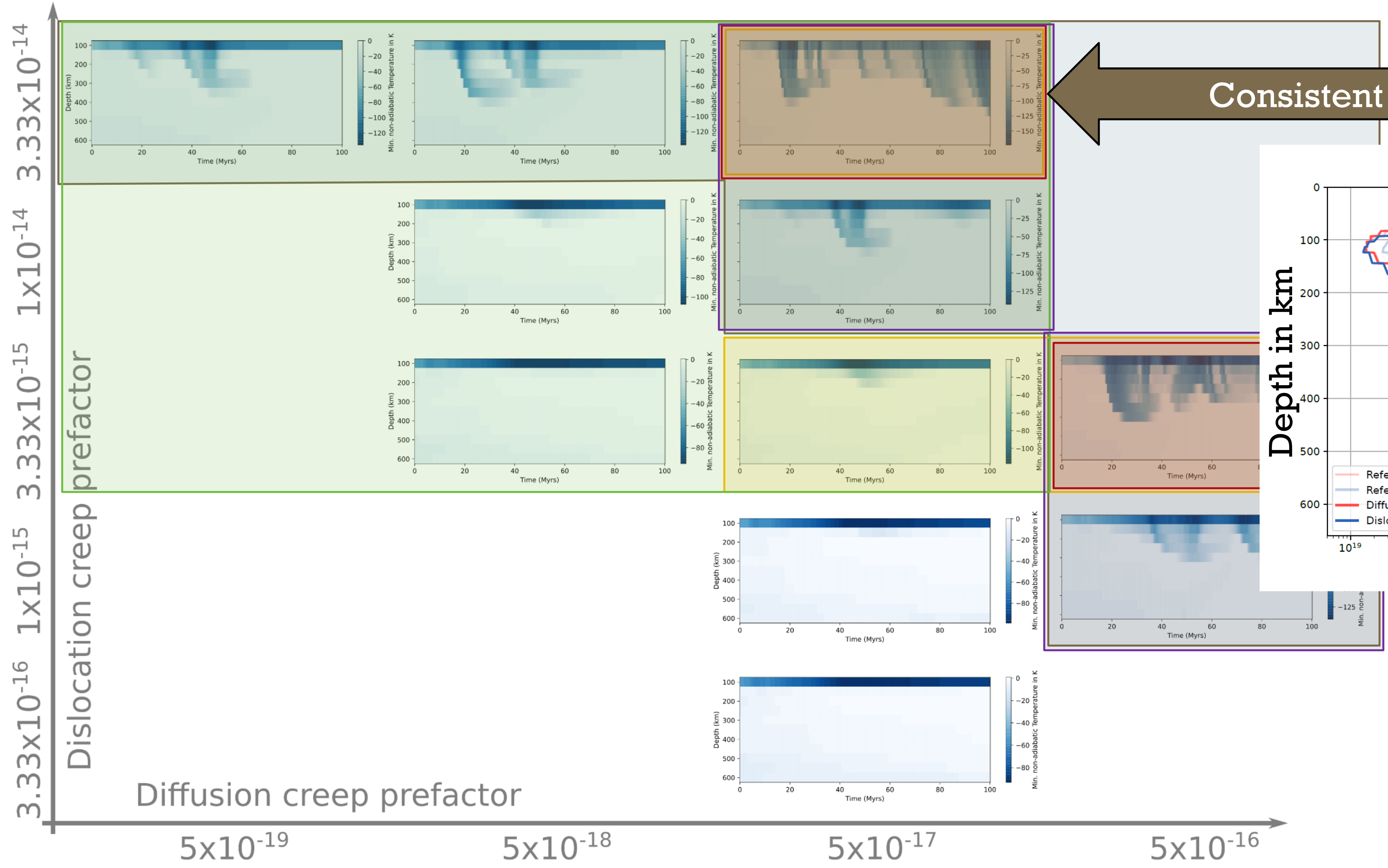
Dynamic topography at the end of the model evolution



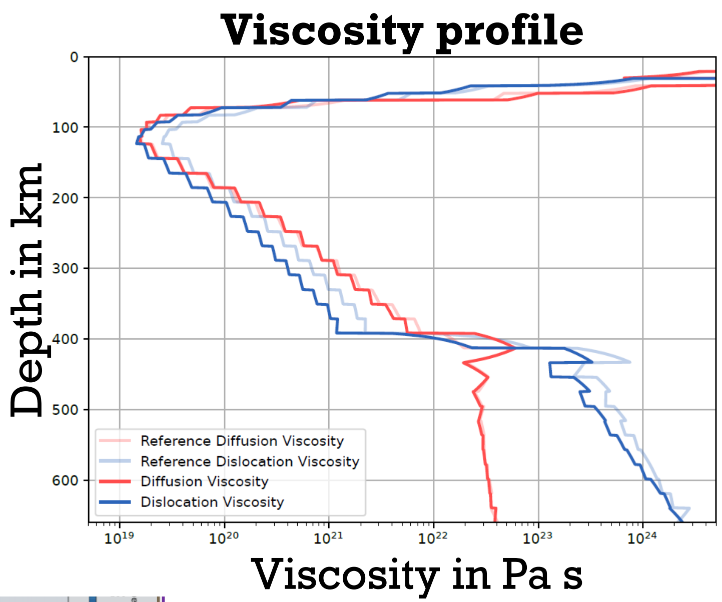


Some models show lineaments at the surface

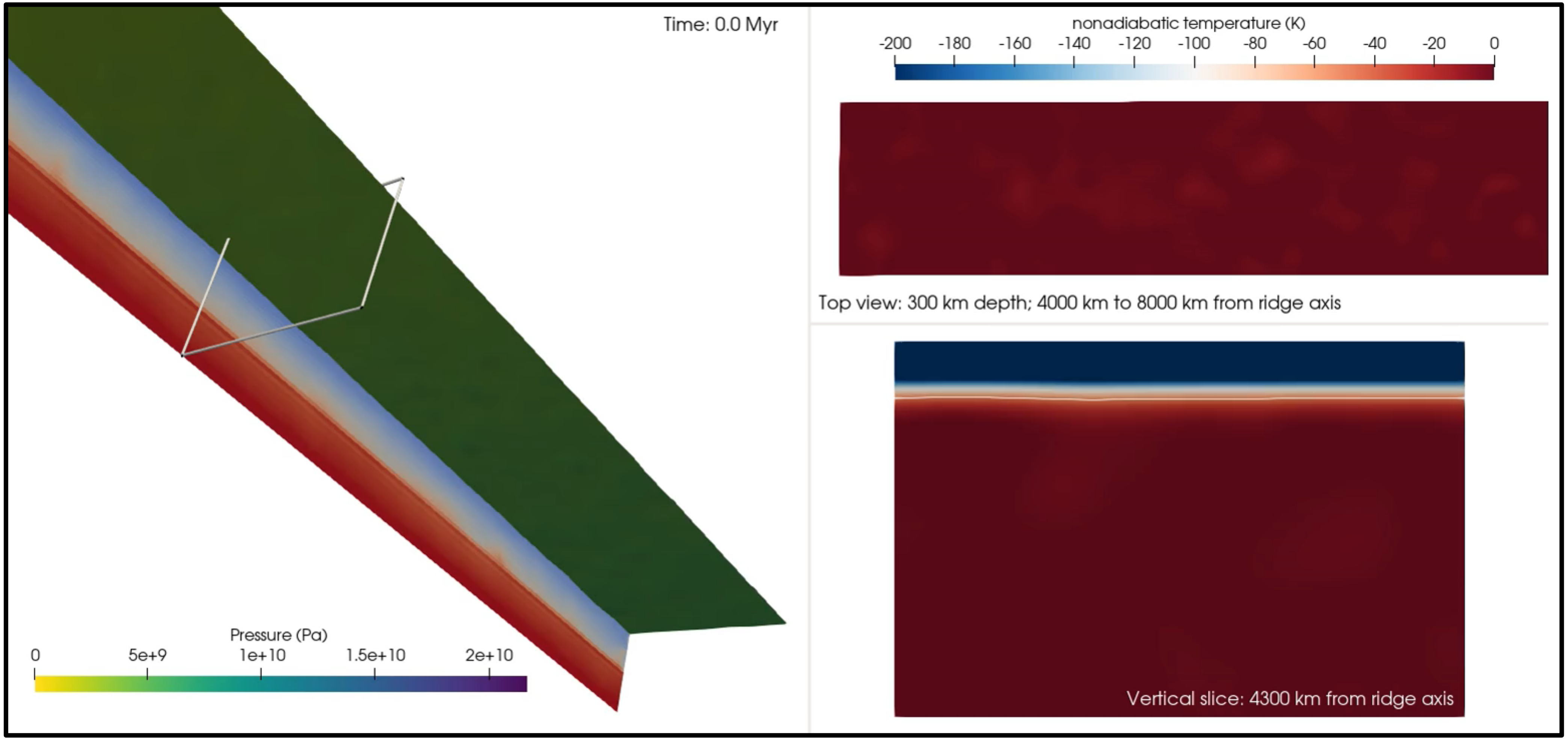
WHICH MODELS ARE CONSISTENT WITH OBSERVATIONS?



Consistent with observations



BEST-FIT MODEL



BREAK: THE VALUE OF RESEARCH SOFTWARE

All of these results are created by modern HPC infrastructure and research software.

How much software did we use for this research?

- ~ 5,000 lines of code per project (modeling, data conversion, statistics and plotting)

How many lines of code did we indirectly use? (ASPECT, deal.II, other scientific libraries)

- ~ 1,700,000 lines of code (ASPECT: 200,000, deal.II: 1,400,000, GeodynamicWorldBuilder: 90,000)

How much did the software development cost?

- ~15$/line of code: ~$3 million (ASPECT), ~$25 million (total)

This software is as expensive as:

- Dozens of PhD projects, or several faculty startup packages,
- Comparable to expensive equipment (mass spectrometer: ~$1 million) or small research vessels (FS Alkor: 33 million DM in 1990)

So scientific software = expensive instruments?

CHALLENGES

OPEN ACCESS Freely available online

PLOS | BIOLOGY

Community Page

Best Practices for Scientific Computing

Greg Wilson[1]*, D. A. Aruliah[2], C. Titus Brown[3], Neil P. Chue Hong[4], Matt Davis[5], Richard T. Guy[6¤], Steven H. D. Haddock[7], Kathryn D. Huff[8], Ian M. Mitchell[9], Mark D. Plumbley[10], Ben Waugh[11], Ethan P. White[12], Paul Wilson[13]

1 Mozilla Foundation, Toronto, Ontario, Canada, **2** University of Ontario Institute of Technology, Oshawa, Ontario, Canada, **3** Michigan State University, East Lansing, Michigan, United States of America, **4** Software Sustainability Institute, Edinburgh, United Kingdom, **5** Space Telescope Science Institute, Baltimore, Maryland, United States of America, **6** University of Toronto, Toronto, Ontario, Canada, **7** Monterey Bay Aquarium Research Institute, Moss Landing, California, United States of America, **8** University of California Berkeley, Berkeley, California, United States of America, **9** University of British Columbia, Vancouver, British Columbia, Canada, **10** Queen Mary University of London, London, United Kingdom, **11** University College London, London, United Kingdom, **12** Utah State University, Logan, Utah, United States of America, **13** University of Wisconsin, Madison, Wisconsin, United States of America

Introduction

Scientists spend an increasing amount of time building and using software. However, most scientists are never taught how to do this efficiently. As a result, many are unaware of tools and practices that would allow them to write more reliable and

error from another group's code was not discovered until after publication [6]. As with bench experiments, not everything must be done to the most exacting standards; however, scientists need to be aware of best practices both to improve their own approaches and for reviewing computational work by others.

Wilson et al, 2014, Plos Biology

- Scientists spend ~30% of their time developing software
- Many important publications had to be retracted or amended due to software bugs
- Software needs as much care as a complex experimental apparatus

If you are new to programming: Wilson et al., 2017: **Good enough practices in scientific computing.**

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

Modeling software

Computational workflows

Training

Community

- **US NSF-funded community-driven** organization (69 national, 21 international affiliate institutions)
- Providing **infrastructure** for **software**
- Distributing **software** and **best practices**
  - Best practices: https://geodynamics.org/software/software-bp
  - Software Template: https://github.com/geodynamics/software_template
- **Training** the next generation of computational geoscientists in virtual and in-person workshops

CONCLUSIONS

Modern numerical methods and rigorous benchmarking provide accurate and reliable geodynamic models.

Combining surface observations with geodynamic models opens additional windows into the properties of the Earth's lithosphere and mantle.

The future of application science relies heavily on research software. Sharing and improving our best practices is essential for building that software.

Thank you for your attention!
Questions or ideas for collaborations?
rgassmoeller@geomar.de

Want to know more?
- Find me on Google Scholar
- My website: gassmoeller.github.io

Publications:

- Gassmoeller et al., Evaluating the accuracy of hybrid finite element/particle-in-cell methods for modelling incompressible Stokes flow. 2019.
- Dannberg, Gassmöller, et al., The importance of grain size to mantle dynamics and seismological observations. 2017.
- Gassmoeller et al. Benchmarking the accuracy of higher order particle methods in geodynamic models of transient flow. 2024.
- Dannberg, Gassmöller et al., Understanding Sub-Lithospheric Small-Scale Convection By Linking Models Of Grain Size Evolution, Mantle Convection and Seismic Tomography. In prep.

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- Computational Infrastructure for Geodynamics (CIG), NSF EAR-1550901, EAR-EAR-2149126
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