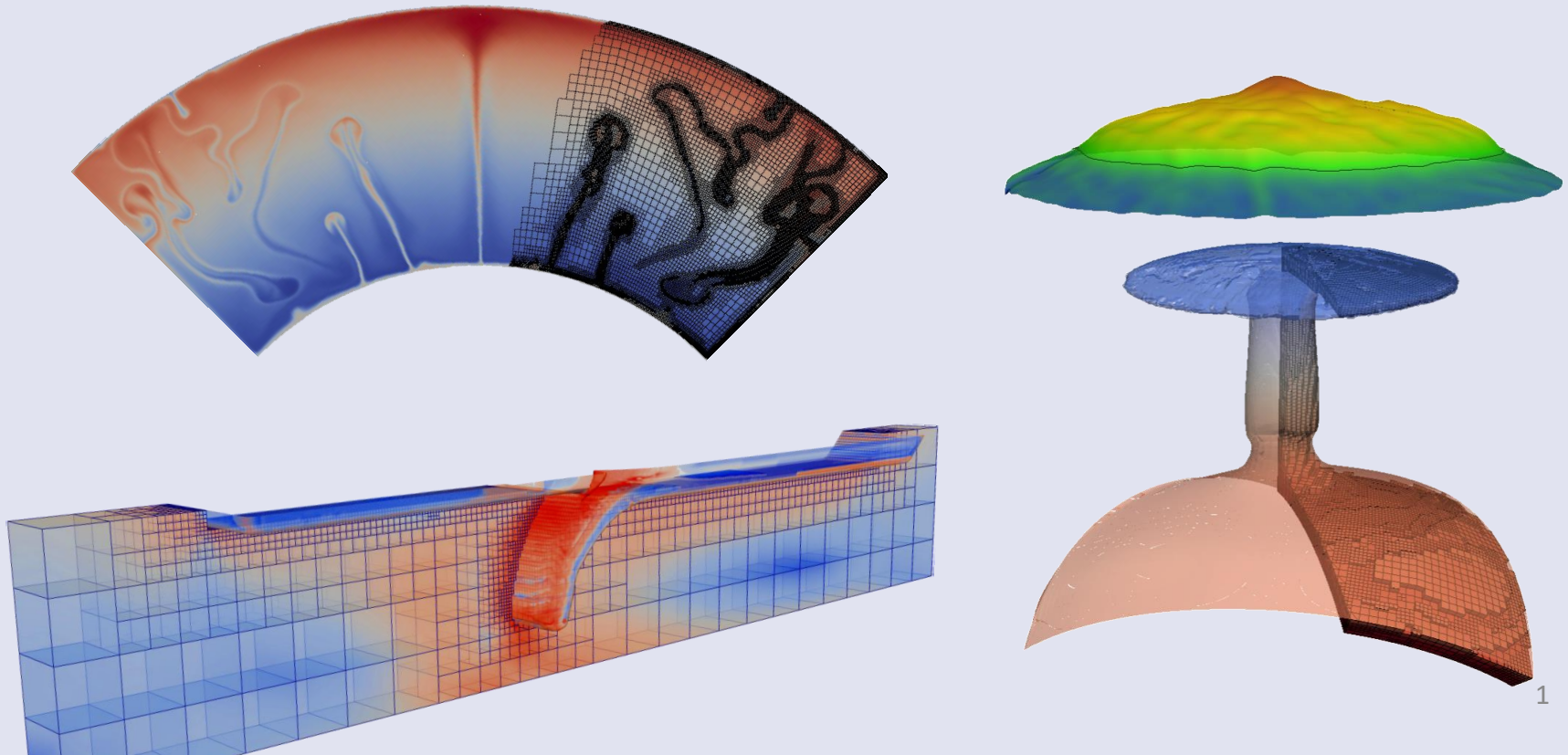


ASPECT

- Advanced Solver for Problems in Earth's Convection -

Rene Gassmüller (with slides by Juliane Dannberg)



- ❖ **Modern numerical methods:**
adaptive mesh refinement, linear and nonlinear solvers, higher-order discretizations, parallel scalability
- ❖ **Modern software development techniques:**
peer code review, continuous integration/testing, extensible plugin architecture
- ❖ **Usability and extensibility:**
manual: 450+ pages, ~40 cookbooks/examples
- ❖ **Building on others' work:**
tested foundation, smaller codebase, automatic improvements
- ❖ **Community:**
open-source (GPL), developed in the open, encourage contributions, be welcoming

- ASPECT is a welcoming community project!
- You are welcome to use ASPECT for your project without obligations (please cite us correctly!), but we can not guarantee suitability for any particular project.
- We encourage your contributions to the main version, which might be useful for other users. Benefits:
 - Compatibility,
 - Data availability,
 - Recognition.
- We transparently collaborate and organize the development of ASPECT on Github:
<https://www.github.com/geodynamics/aspect>,
and you are welcome to contribute!

Credits

Website and manual:

aspect.geodynamics.org

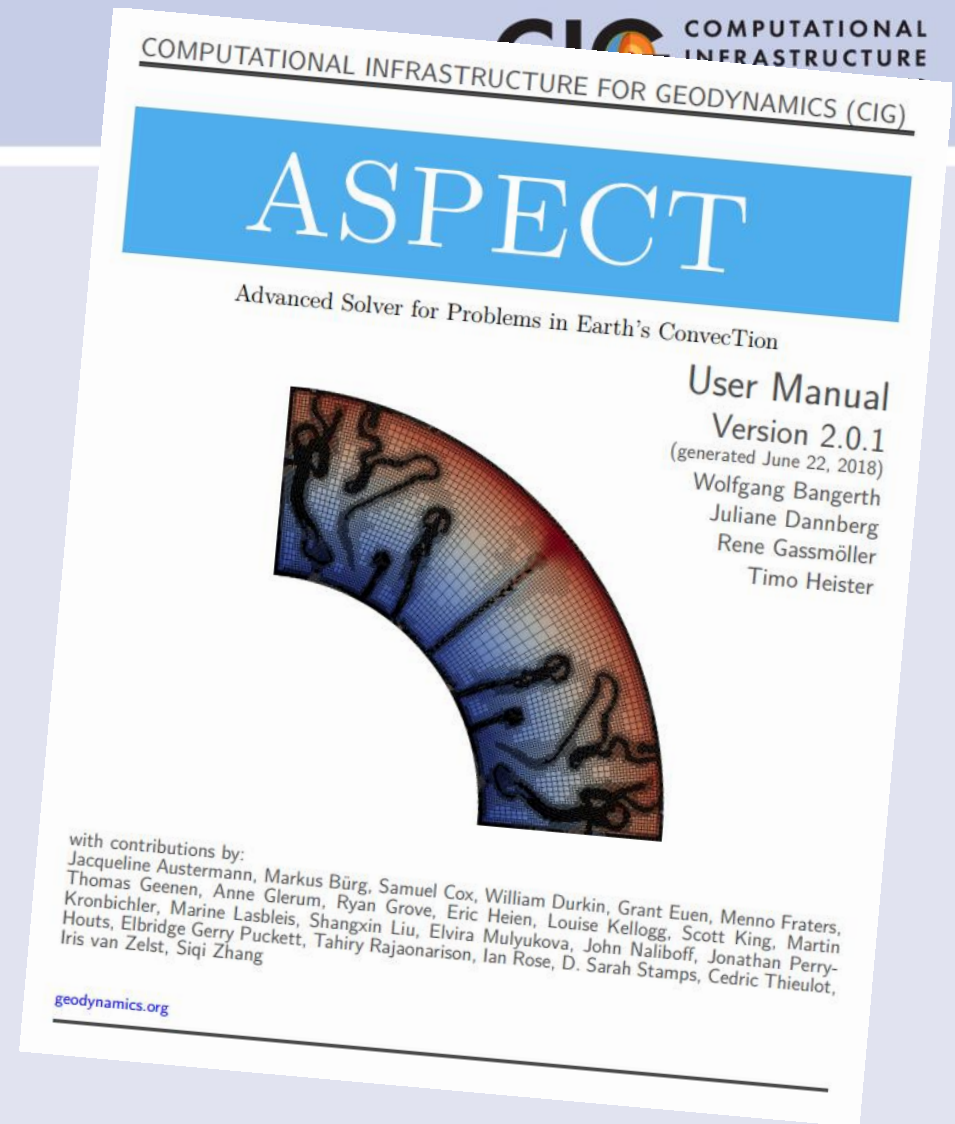
Maintainers:

Wolfgang Bangerth,
Juliane Dannberg,
Timo Heister, Rene Gassmöller
+4 principal developers

Contributors: many more (~45)

Publications: (~30)

- Kronbichler, Heister, Bangerth:
“High Accuracy Mantle Convection Simulation through Modern Numerical Methods”.
Geophysical Journal International, 2012.
- Heister, Dannberg, Gassmoeller, Bangerth: “High Accuracy Mantle Convection Simulation through Modern Numerical Methods. II: Realistic Models and Problems”. *Geophysical Journal International*, 2017.



- ASPECT is installed for the “geodynamics” user in the VM
- Basic usage of ASPECT is specified through a parameter text file (e.g. tutorial.prm)
- The parameter file is used by the simulation to determine the discretization, parameters, initial conditions, boundary conditions, etc.
- By the end of this tutorial, you will be able to:
 1. Run aspect from the command line.
 2. Understand the basic layout of the parameter files that are used to control Aspect simulations.
 3. Be able to visualize the generated output in ParaView.
 4. Understand the concept of a buoyancy ratio, and the interaction between thermal and chemical buoyancy in mantle convection.

1. Open a terminal (ctrl+alt+t)

2. Change to the tutorial directory:

```
cd Desktop/renegassmoeller-aspect
```

3. Start ASPECT with the tutorial parameter file:

```
mpirun -np 2 aspect-release \  
driven_thermochemical_convection.prm
```

4. Open the output in a new terminal (ctrl+alt+t):

```
cd Desktop/renegassmoeller-aspect  
leafpad output-driven_thermochemical_convection/log.txt
```

Look at log.txt

- Numerical models generally consist of several key components:
 1. The rules (e.g. equations) for the model
 2. The boundary conditions
 3. The initial state
 4. Parameters for material properties
 5. The discretization of the model (the mesh)
 6. The output files
- We will go through the parameter file and look at these components:

```
cd Desktop/rene_gassmoeller-aspect  
leafpad driven_thermochemical_convection.prm
```


Look at parameter file

Equations

$$-\nabla \cdot \left[2\eta \left(\varepsilon(\mathbf{u}) - \frac{1}{3}(\nabla \cdot \mathbf{u})\mathbf{1} \right) \right] + \nabla p = \rho \mathbf{g}$$

Force balance

Shear stress in rock + Pressure gradient = Buoyancy force

Equations

Shear stress in rock + Pressure gradient = Buoyancy force Force balance

$\nabla \cdot (\rho \mathbf{u}) = 0$ Conservation of mass

Change of mass in a given volume + Inflow/outflow of mass = 0

Equations

Stresses in the rock + Pressure gradient = Buoyancy force Force balance

Change of mass in a given volume + Inflow/outflow of mass = 0 Conservation of mass

$$\rho C_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) - \nabla \cdot k \nabla T = \rho H$$

Conservation of energy

$$+ 2\eta \left(\varepsilon(\mathbf{u}) - \frac{1}{3}(\nabla \cdot \mathbf{u})\mathbf{1} \right) : \left(\varepsilon(\mathbf{u}) - \frac{1}{3}(\nabla \cdot \mathbf{u})\mathbf{1} \right)$$

$$+ \alpha T \mathbf{u} \cdot \nabla p$$

$$+ \rho T \cdot \Delta S \frac{DX}{Dt}$$

Change of energy over time + Advection + Heat conduction = Heat generation (caused by a number of processes)

Equations

$$-\nabla \cdot \left[2\eta \left(\varepsilon(\mathbf{u}) - \frac{1}{3}(\nabla \cdot \mathbf{u})\mathbf{1} \right) \right] + \nabla p = \rho \mathbf{g}$$

Momentum equation

$$\nabla \cdot (\rho \mathbf{u}) = 0$$

Conservation of mass

$$\rho C_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) - \nabla \cdot k \nabla T = \rho H$$

Conservation of energy

$$+ 2\eta \left(\varepsilon(\mathbf{u}) - \frac{1}{3}(\nabla \cdot \mathbf{u})\mathbf{1} \right) : \left(\varepsilon(\mathbf{u}) - \frac{1}{3}(\nabla \cdot \mathbf{u})\mathbf{1} \right)$$

$$+ \alpha T \mathbf{u} \cdot \nabla p \quad + \rho T \cdot \Delta S \frac{DX}{Dt}$$


$$\frac{\partial c_i}{\partial t} + \mathbf{u} \cdot \nabla c_i = 0$$

Advection of compositional fields

\mathbf{u}	velocity	$\frac{m}{s}$
p	pressure	Pa
T	temperature	K
$\varepsilon(\mathbf{u})$	strain rate	$\frac{1}{s}$
η	viscosity	Pa · s

ρ	density	$\frac{kg}{m^3}$
\mathbf{g}	gravity	$\frac{m}{s^2}$
C_p	specific heat capacity	$\frac{J}{kg \cdot K}$
k	thermal conductivity	$\frac{W}{m \cdot K}$
H	intrinsic specific heat production	$\frac{W}{kg}$

Visualizing Results with ParaView

- To visualize the simulation results, we will use ParaView 
- ParaView is an open-source program for visualization of large data sets
- It is installed on the virtual machine, open it now by typing “paraview” in a new terminal
- ParaView supports visualization tools such as isosurfaces, slices, streamlines, volume rendering, and other complex visualization techniques

Visualization with ParaView

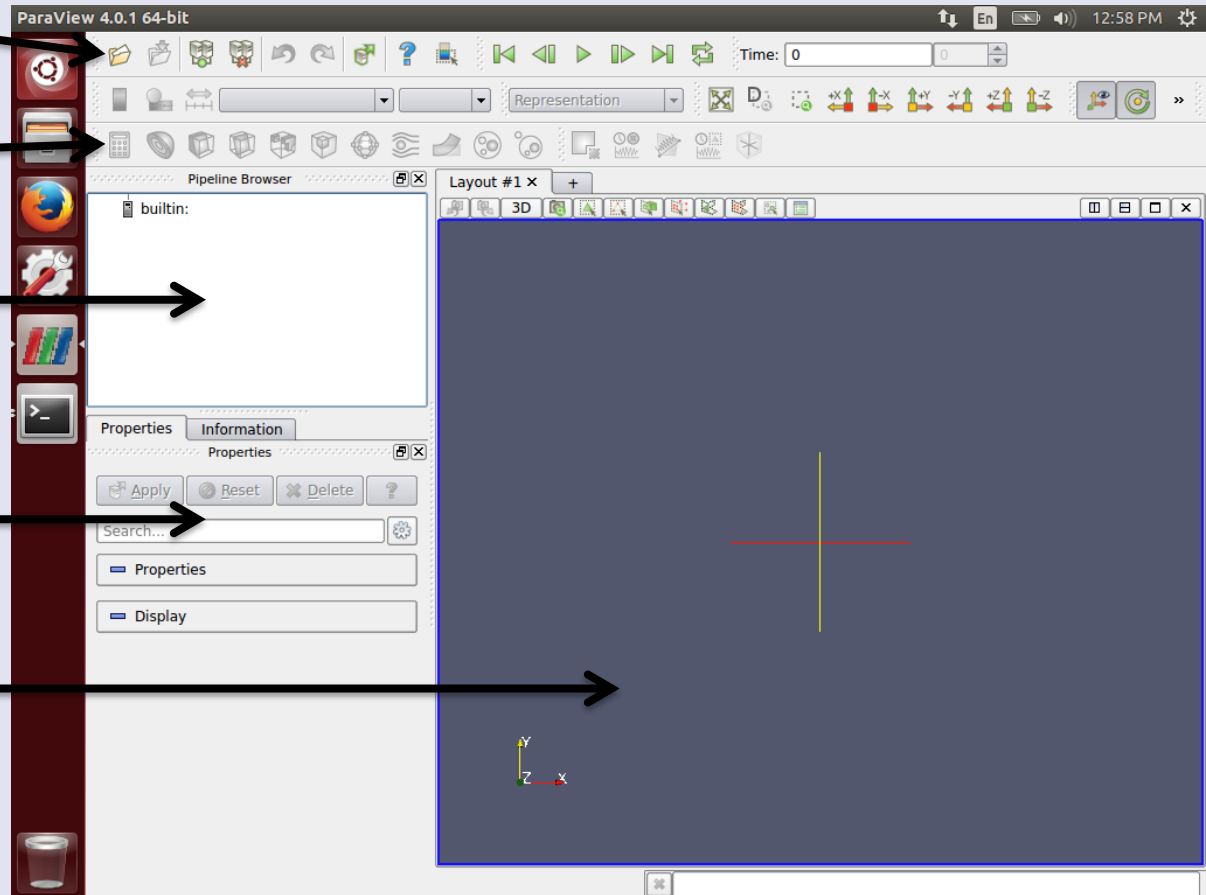
Open file


Toolbars

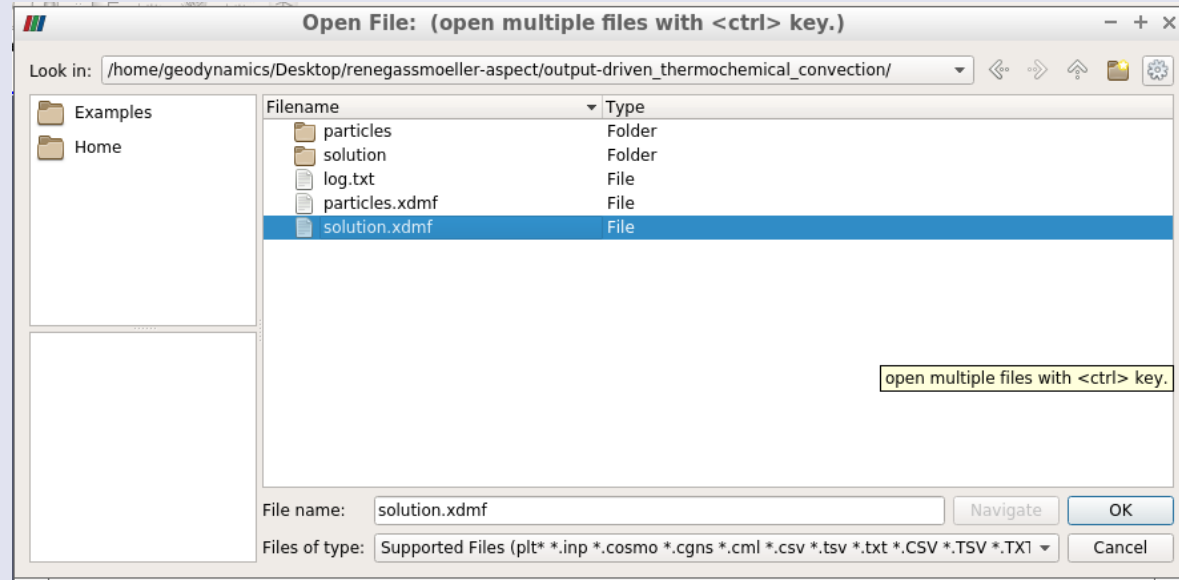
Pipeline Browser

Object Inspector

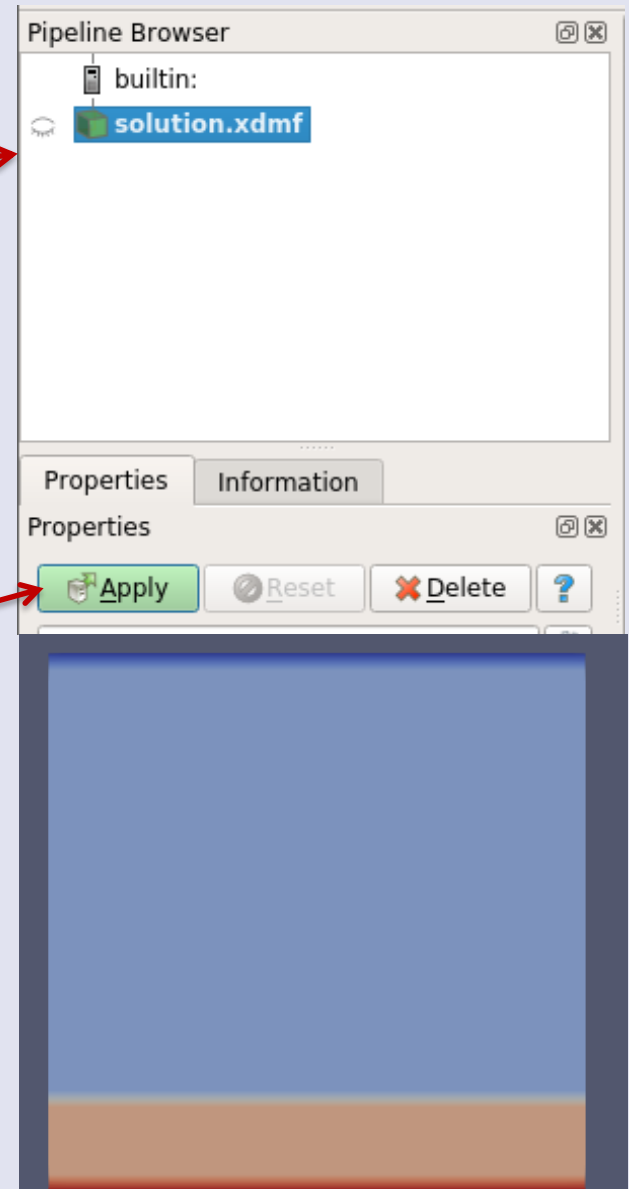
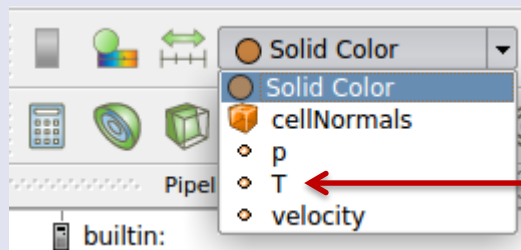
2D/3D View



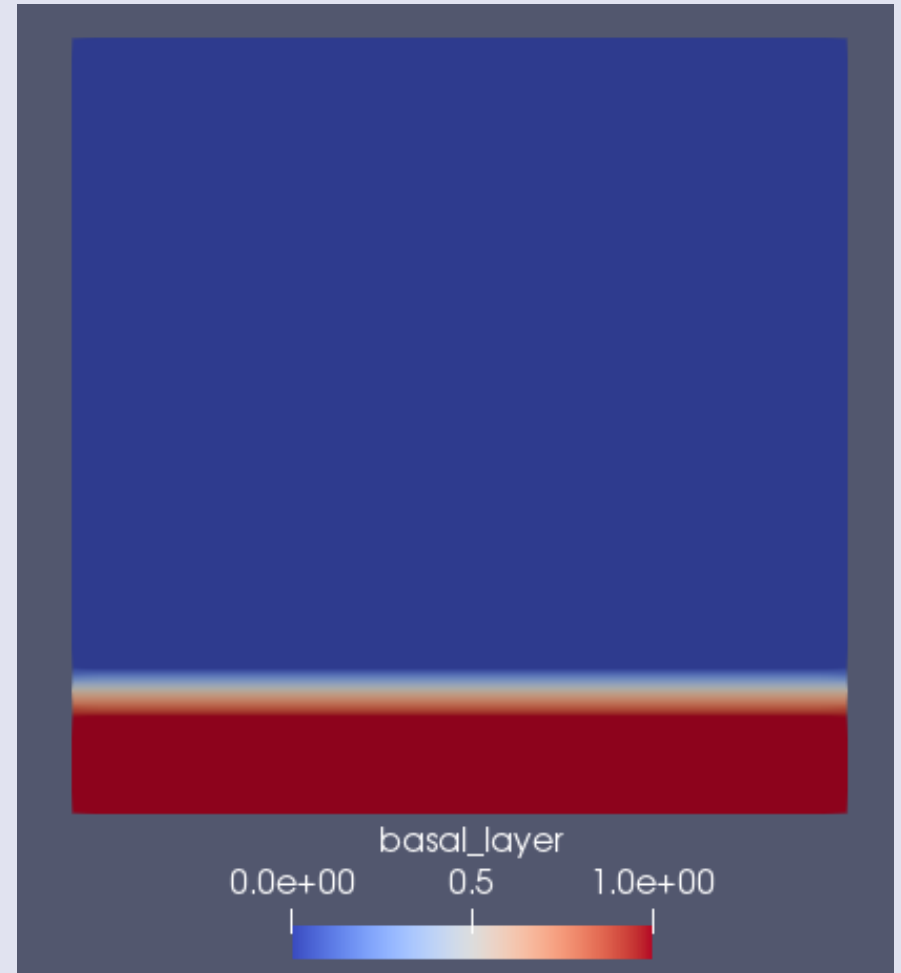
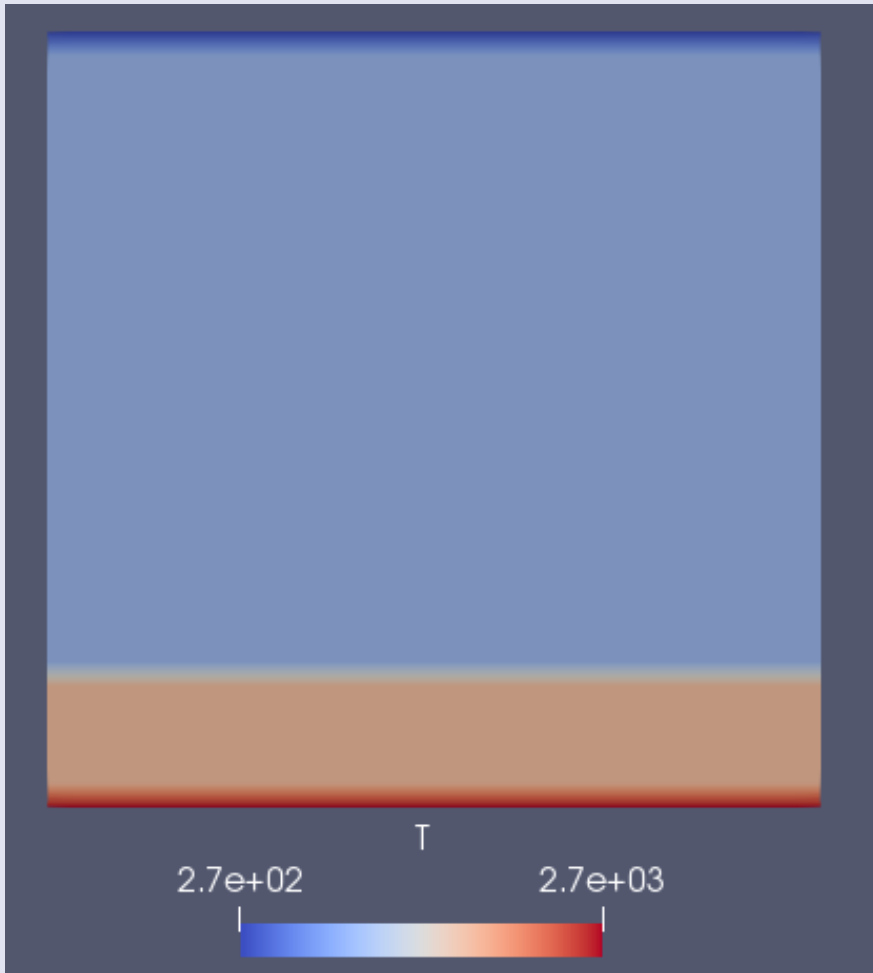
- Start by opening solution.xdmf which was created by running ASPECT
- You can choose “Open” from the File menu or use the Open icon  in the toolbar
- The file is in `/home/geodynamics/Desktop/renegeassmoeller-aspect/output-driven_thermochemical_convection`



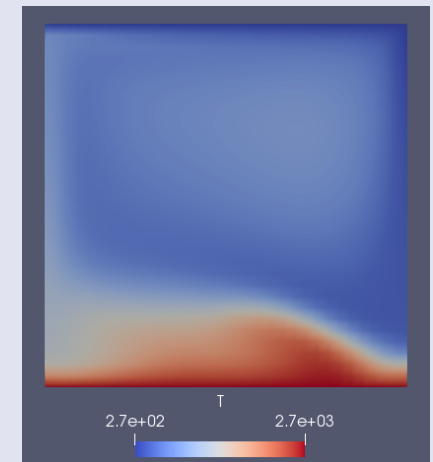
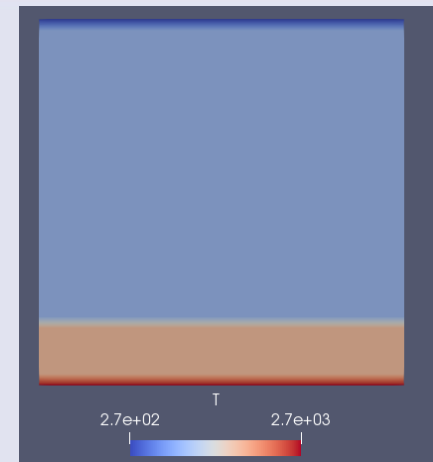
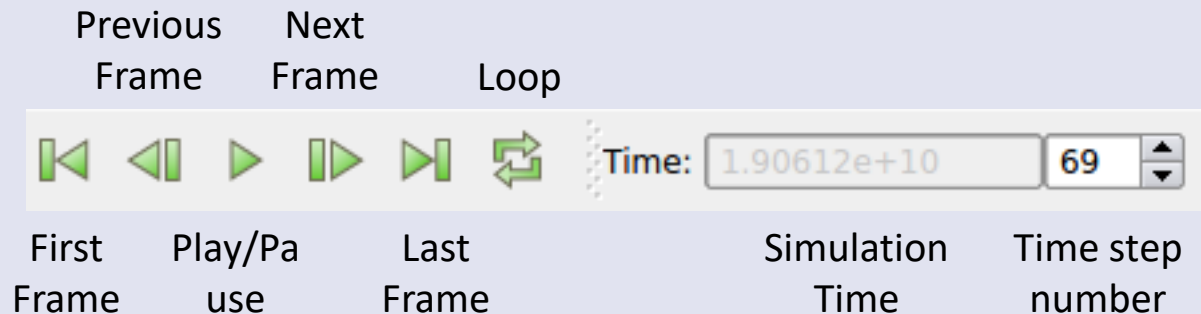
- The file will appear in the pipeline browser
 - Make sure it is solution.xdmf
- Click “Apply” to show the field in the view area
 - Select “T” in the toolbar to show the temperature field



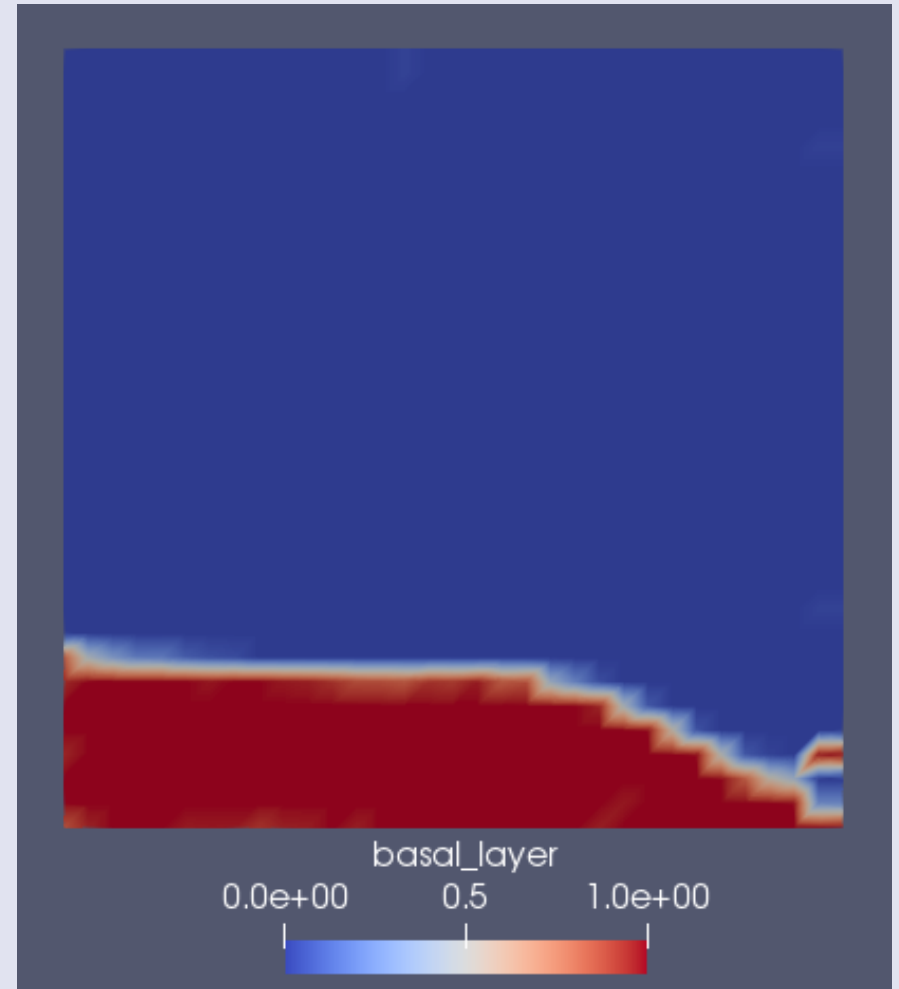
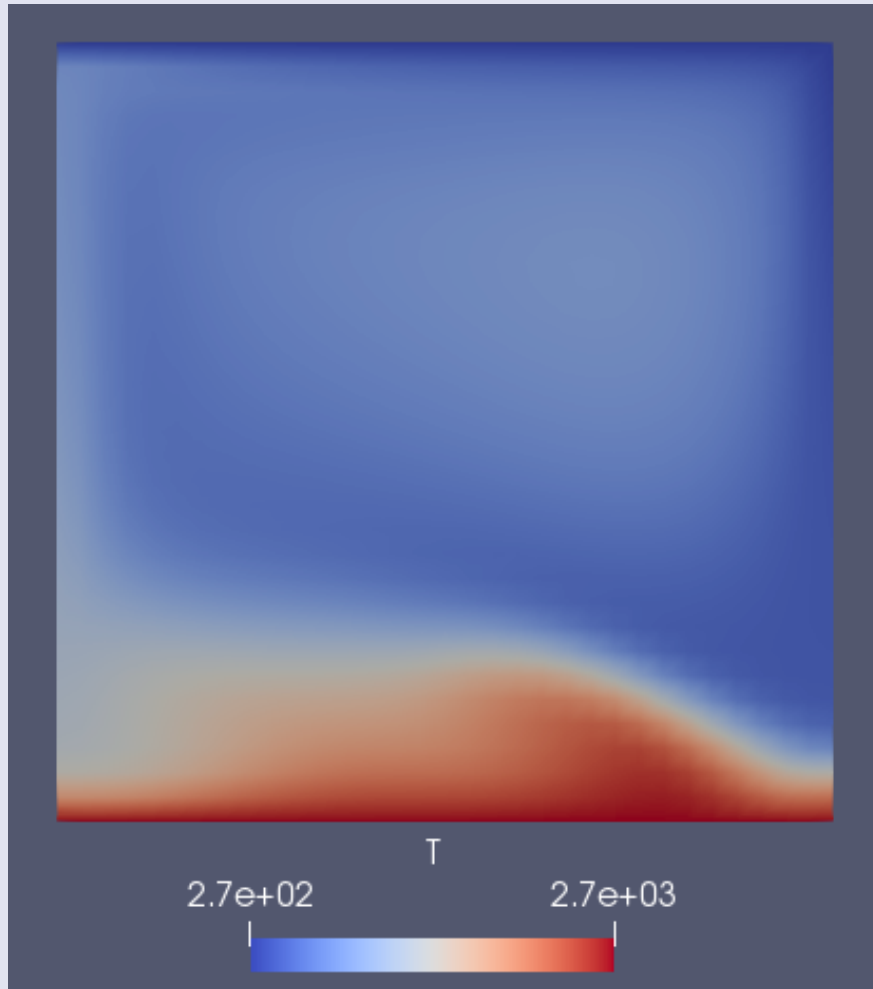
Does the initial state look ok?



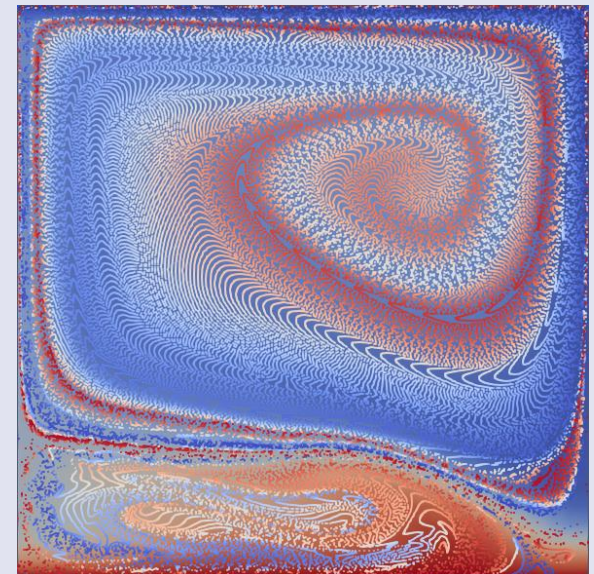
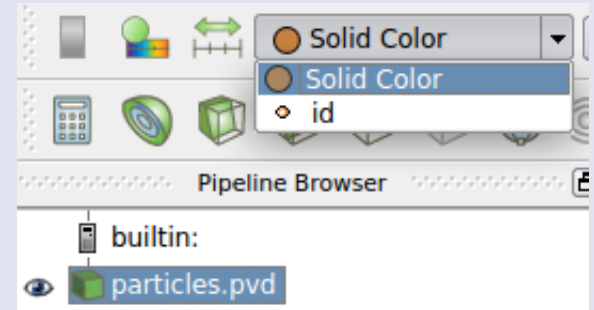
- The top toolbar has buttons to change the time, shown below
 - Click the play button and watch how the temperature field changes
 - Near the end, is the temperature field static? Is the velocity field static? Is material moving?



What is the final state?



- Open the file particles.xdmf and click “Apply”
 - The tracer particles from the simulation now appear on the temperature field
 - Click play again to see how material is flowing with the particles
 - Even when the temperature field is static, is material flowing?
 - What happens to the basal layer?



Temperature field with
particles

Preliminary conclusions:

1. The cold downwelling material deforms the dense basal layer.
2. The temperature in the basal layer remains hotter than in the material above.
3. Layer and background material are convecting.
4. Very little material from the basal layer is entrained into the convection above.

What controls layer stability?

- Heating from the core-mantle boundary
- Density contrast of layer
- Other factors (heating in layer, viscosity contrast, numerical errors, mechanical mixture)

What controls layer stability?

Group	Parameter	Old value	New value
all	Output directory	output- driven_thermochemi- cal_convection	output-stability_test
1	Bottom temperature Gravity/Magnitude	2700 10	3700 7
2	Density differential for compositional field 1	150	105
3	All of the above	2700 10 150	3700 7 210

- Change parameter file (don't forget to save changes):

```
cd Desktop/renegeassmoeller-aspect
```

```
leafpad driven_thermochemical_convection.prm
```

What controls layer stability?

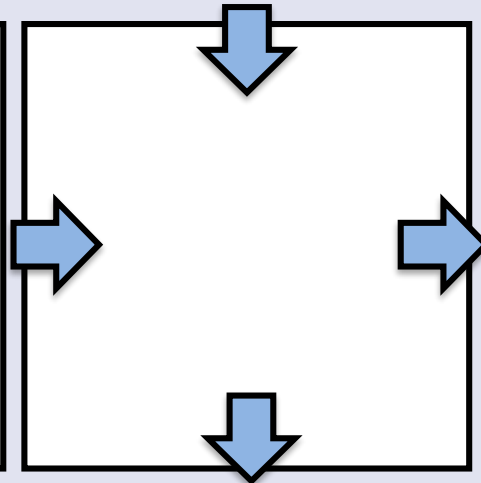
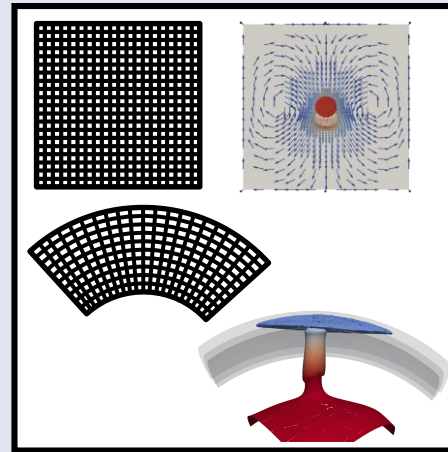
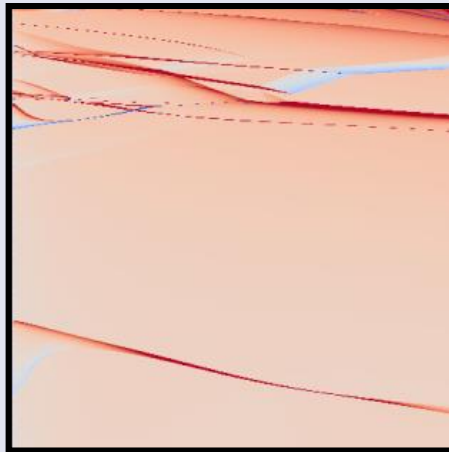
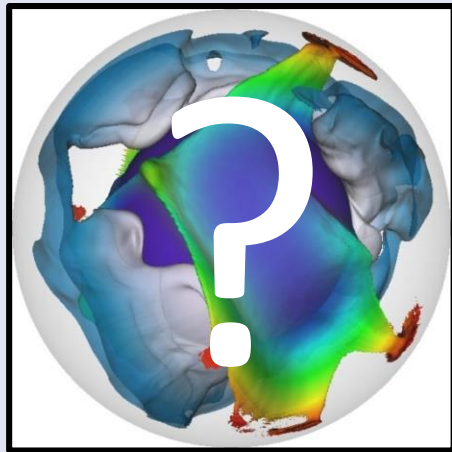
Group	Parameter	Old value	New value
all	Output directory	output- driven_thermochemi- cal_convection	output-stability_test
1	Bottom temperature Gravity/Magnitude	2700 10	3700 7
2	Density differential for compositional field 1	150	105
3	All of the above	2700 10 150	3700 7 210

- Rerun model:

```
mpirun -np 2 aspect-release \  
driven_thermochemical_convection.prm
```

While we wait ...

The philosophy of a model



What is a geodynamic model?

- Models are mathematical simplifications of the Earth
- „All models are wrong, but some are useful“
--George Box
- We can use them to
 - Formulate and test hypotheses
 - Understand processes/interactions
 - Make predictions given the model assumptions (forward model)
 - Find the most plausible model given the observations (inverse model)

How to set up your model:

- I. Decide on the question you want to answer/the theory you want to test
- II. What has to be included in the model to answer this question and what can be simplified?
 - Select equations/setup of a model accordingly
- III. What is the best tool to use for this setup?
- IV. Verification & Validation (not covered today)

Always ask:

What can this model tell us?

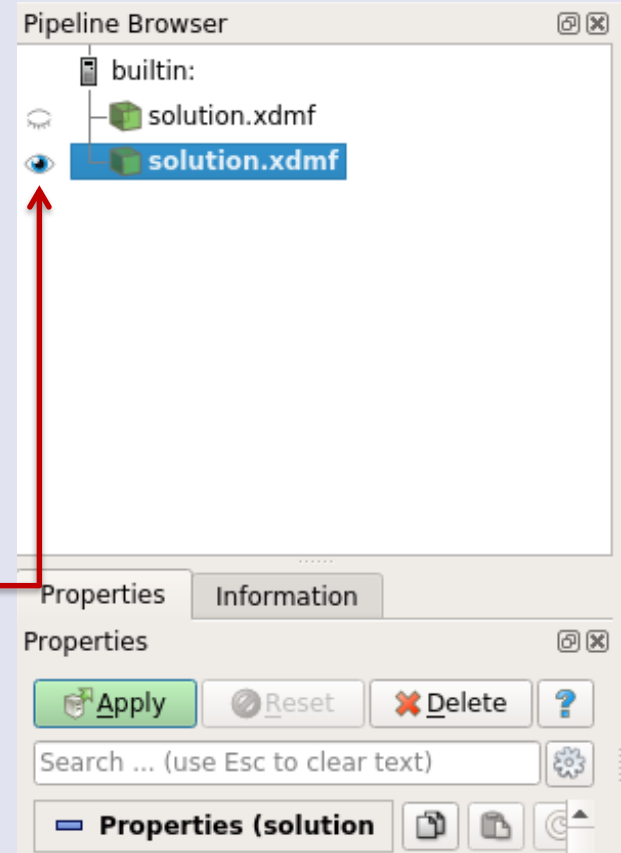
What our model can tell us:	What our model can not do/test:
Influence of density contrasts on stability	Simulate Earth
Influence of temperature contrast on stability	Influence of radiogenic heat generation
Investigate the interaction between these parameters	Influence of viscosity contrasts between layer and background
Spot deficiencies of the used advection methods	Behavior in consistently generated flow patterns (plumes, slabs)
Introduce the concept of a buoyancy ratio	Behavior in realistic geometries (3D, spherical shell)

What determines the stability?

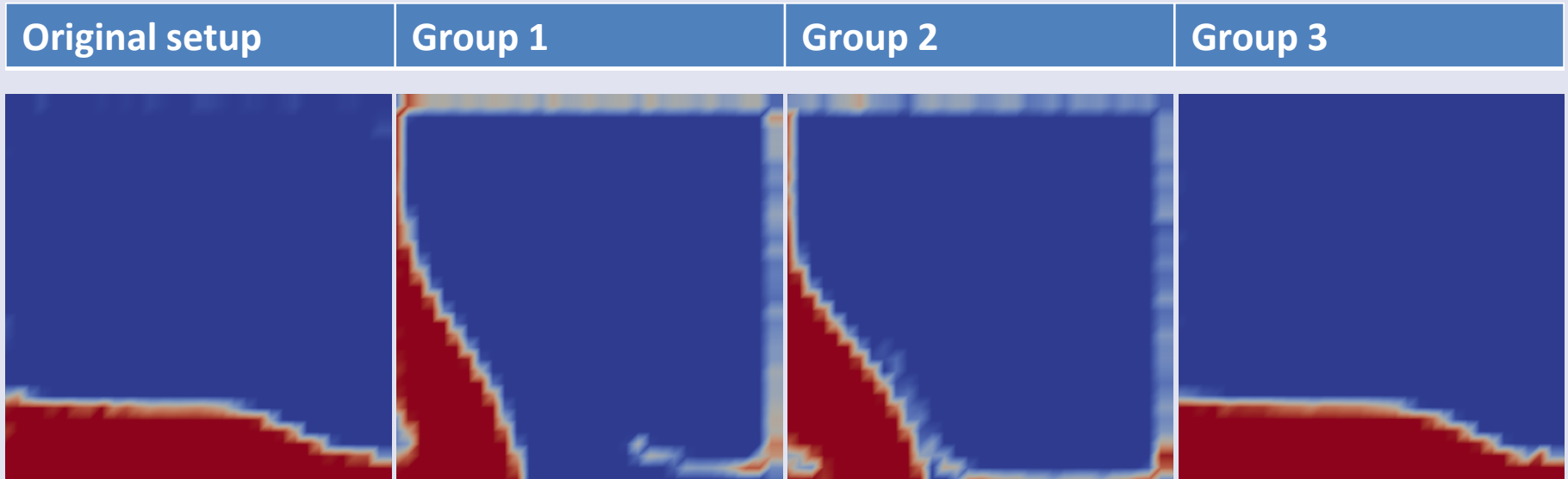
Group	Parameter	Old value	New value
all	Output directory	output- driven_thermochemi- cal_convection	output-stability_test
1	Bottom temperature Gravity/Magnitude	2700 10	3700 7
2	Density differential for compositional field 1	150	105
3	All of the above	2700 150	3700 210

- Visualize your model results in Paraview

- You can load multiple files at the same time
 - Load the original solution and your modified solution
- You can control which solution is shown using the little ‘eye’ icon next to solution.xdmf
- Compare the results of the field ‘basal_layer’ after half of the model runtime



Model results (at 2.5 Gy)



- Results of Group 1 and 2, and results of Group 3 and original setup look suspiciously similar
- Modifying thermal and chemical density contrast leads to similar results, and can cancel each other

- The ratio of thermal and chemical density contrast (the buoyancy ratio ***B***) determines the stability of a dense layer

$$B = \Delta\rho_{ch} / (\rho_0\alpha_0\Delta T)$$

Group	Original	Group 1	Group 2	Group 3
Buoyancy ratio	~0.91	~0.65	~0.65	~0.91

- Small differences in ***B*** accumulate over time and can lead to diverging results (compare end result of Group 1 and 2), why is that?

ASPECT can run in debug or optimized mode:

- DEBUG mode:
 - lots of internal checks to verify correctness of algorithms in deal.II, ASPECT, and user-provided plugins
 - no compiler optimizations to make debugging simpler, slow
 - always run models in debug mode first
- OPTIMIZED (or RELEASE) mode:
 - most internal checks are switched off
 - use available compiler optimizations
 - fast: about 4-10 times faster
 - always run production models in release mode (after testing in debug mode)
- **aspect** in your VM links to **debug** mode,
aspect-release to **release** mode

How to ...

... find available input options?

... see how things work?

... know if someone already did something?

... implement something new?

- Appendix of manual
- Look through included cookbooks, benchmarks, tests and the manual
- Ask on mailing list
- Start from a similar model
- Discuss your ideas with us (no obligations)

Where to find more ASPECT?

Website

aspect.geodynamics.org

Github

github.com/geodynamics/aspect

Mailing list

aspect-devel@geodynamics.org

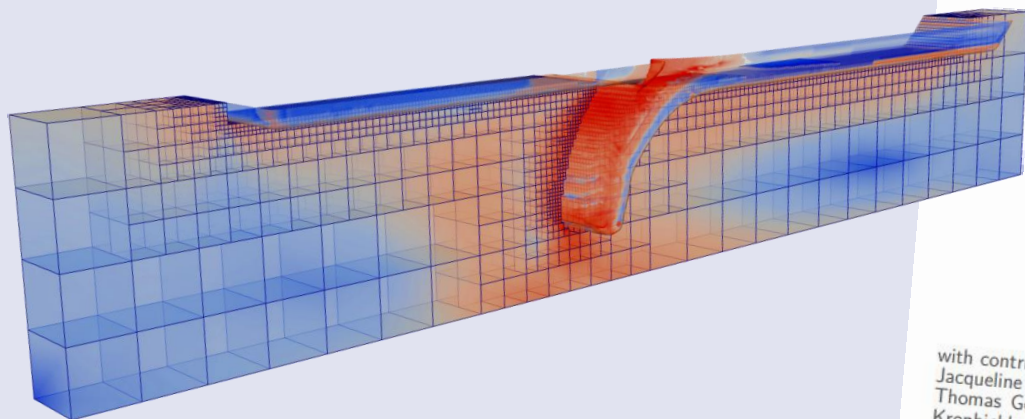
Subscribe at:

<https://geodynamics.org/cig/about/ mailing-lists/>

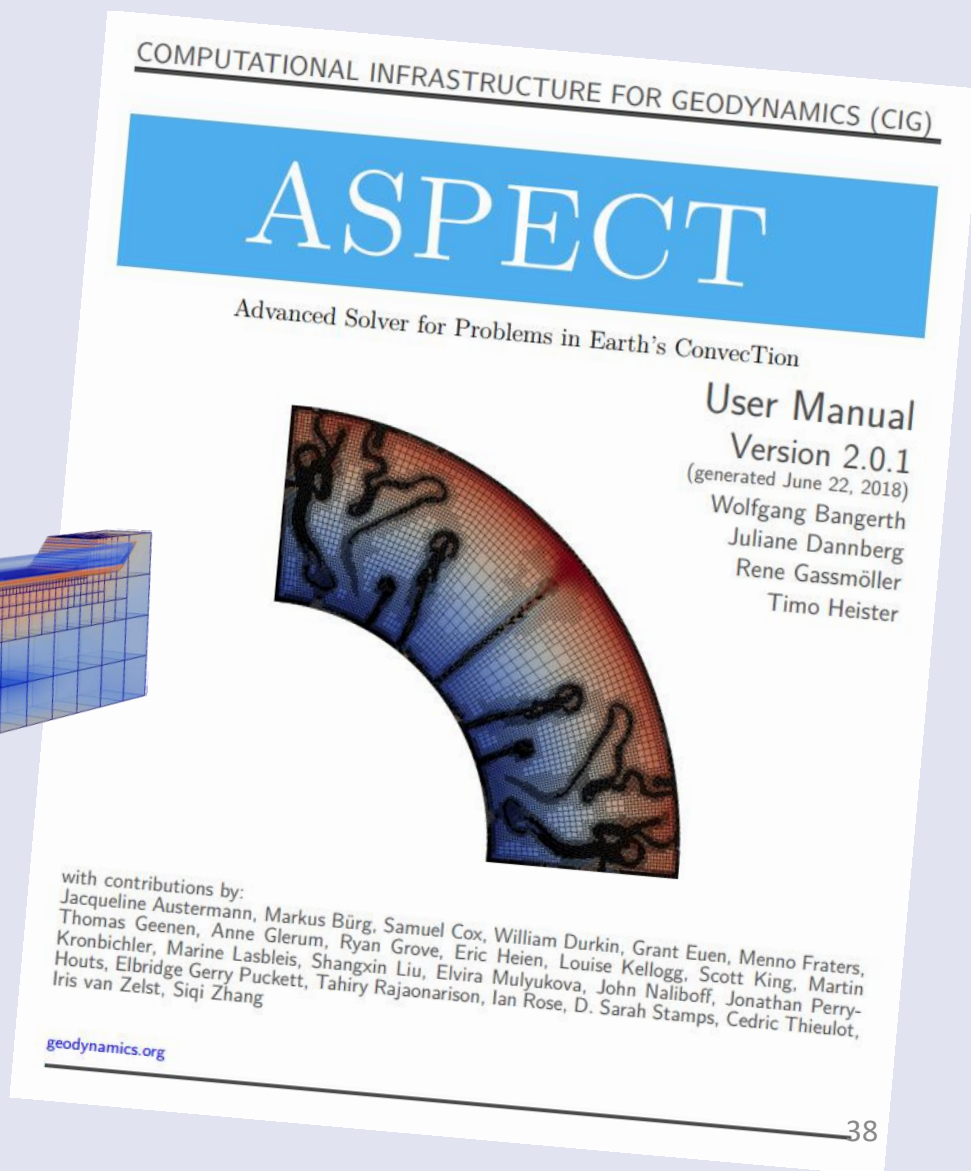
- Announcements, publications, news
- New features, bug reports, contributions
- Questions, discussions, newsletter, meeting other users

Time for your model ideas!

THANK YOU!



More information:
aspect.geodynamics.org



How to learn more ASPECT?

Video Tutorials at
aspect.geodynamics.org

Manual / Cookbooks
[aspect/cookbooks](http://aspect/geodynamics.org/cookbooks)

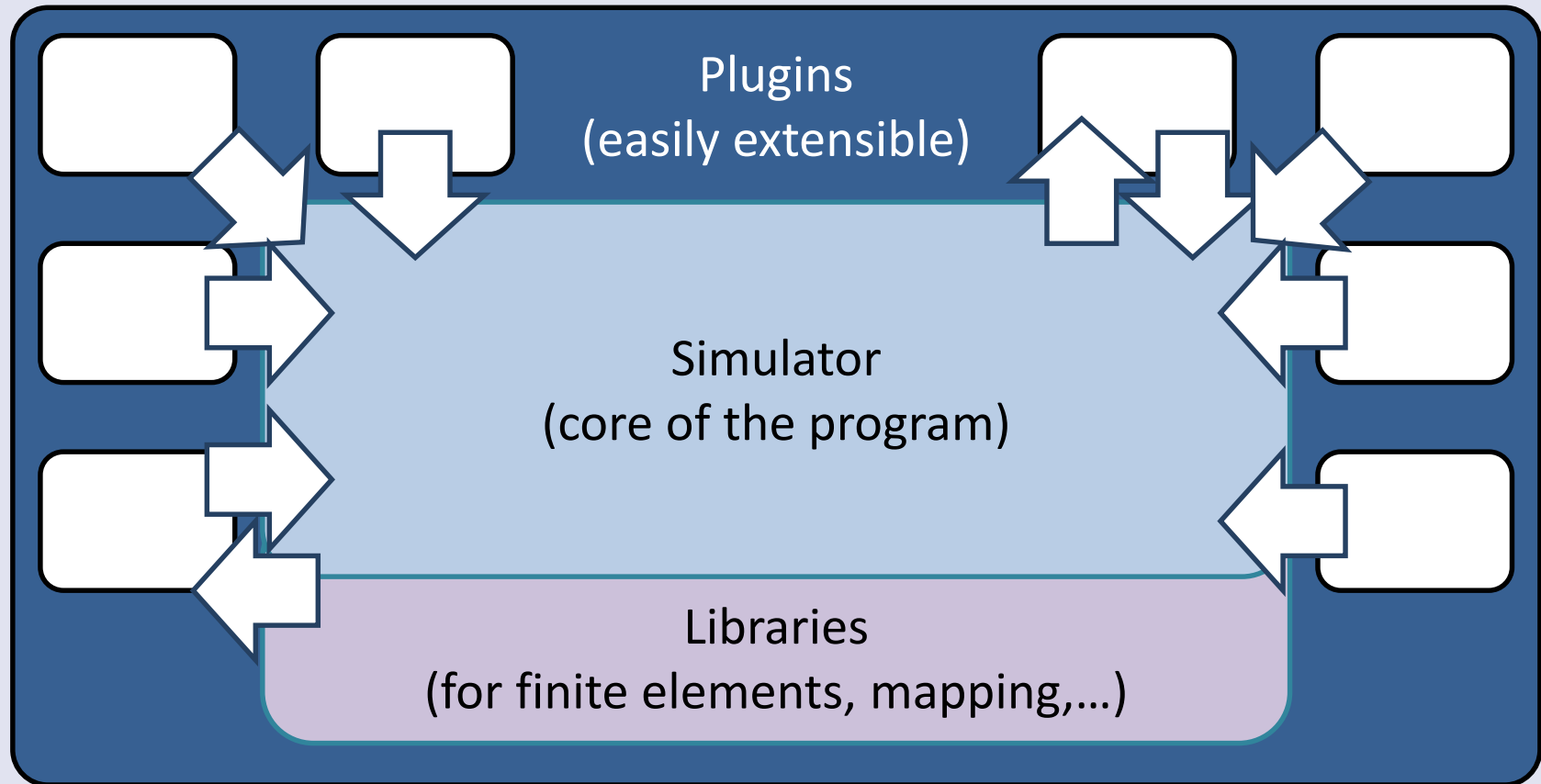
Publications
aspect.geodynamics.org

Benchmarks
[aspect/benchmarks](http://aspect/geodynamics.org/benchmarks)

Tests
[aspect/tests](http://aspect/geodynamics.org/tests)

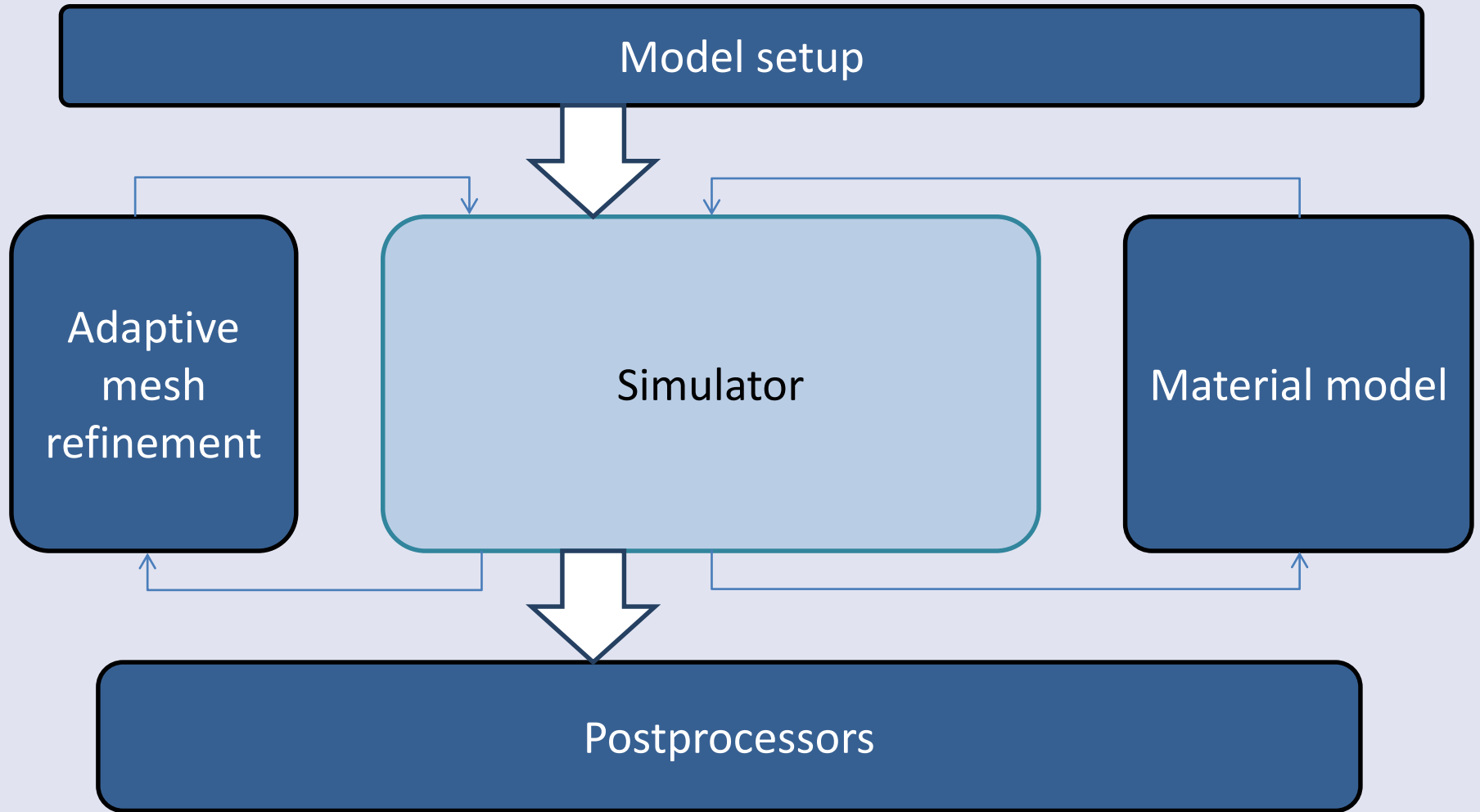
Increasingly detailed ↑

↑ Increasingly many ↓

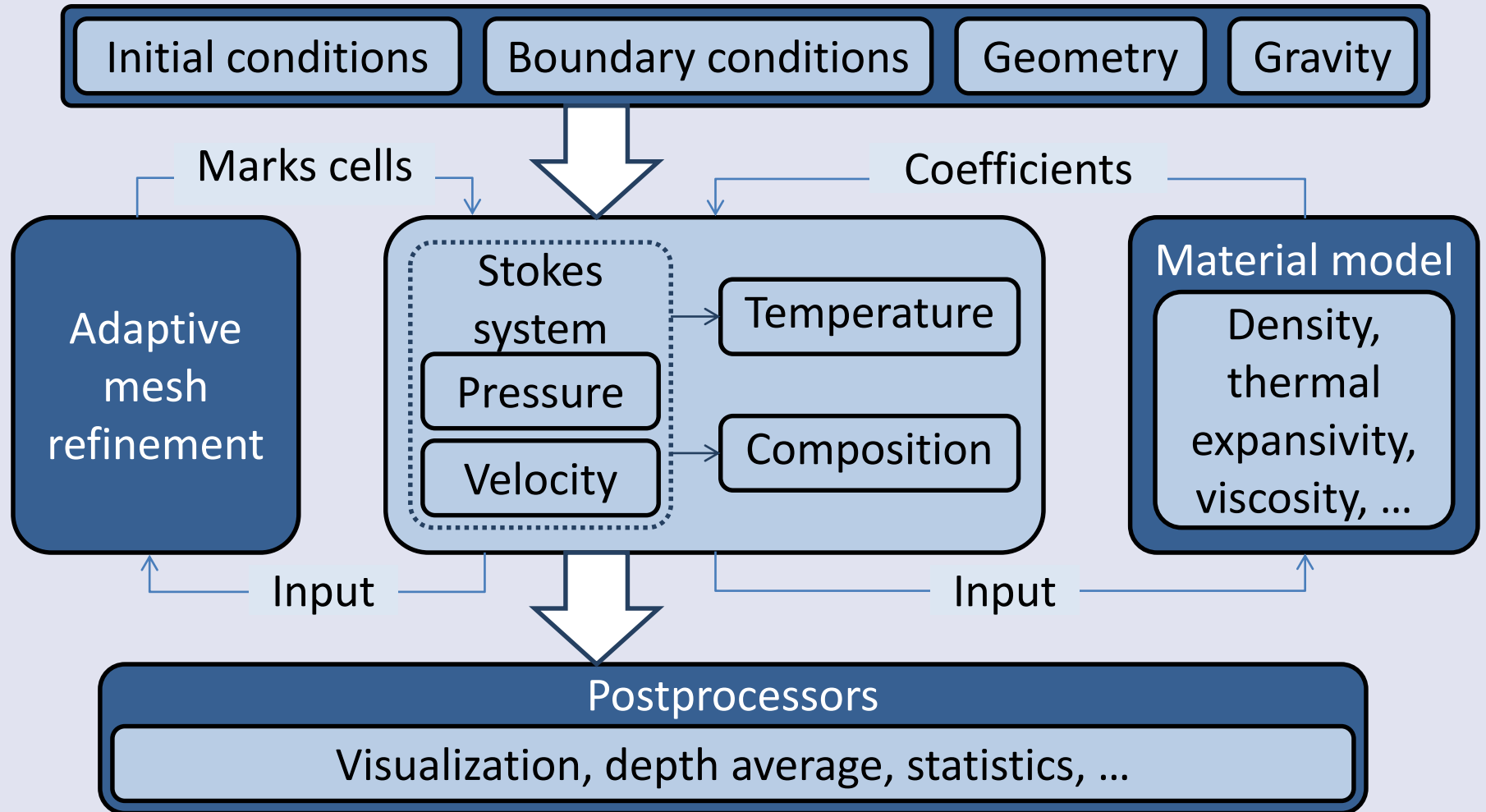


- ASPECT is written in C++ and uses object-oriented design, and advanced language features to keep it manageable despite its size
- You need to understand C++, and deal.II (our main library) if you change the Simulator class / core part
- Most of the plugins are much simpler to understand, and all you need to deal with

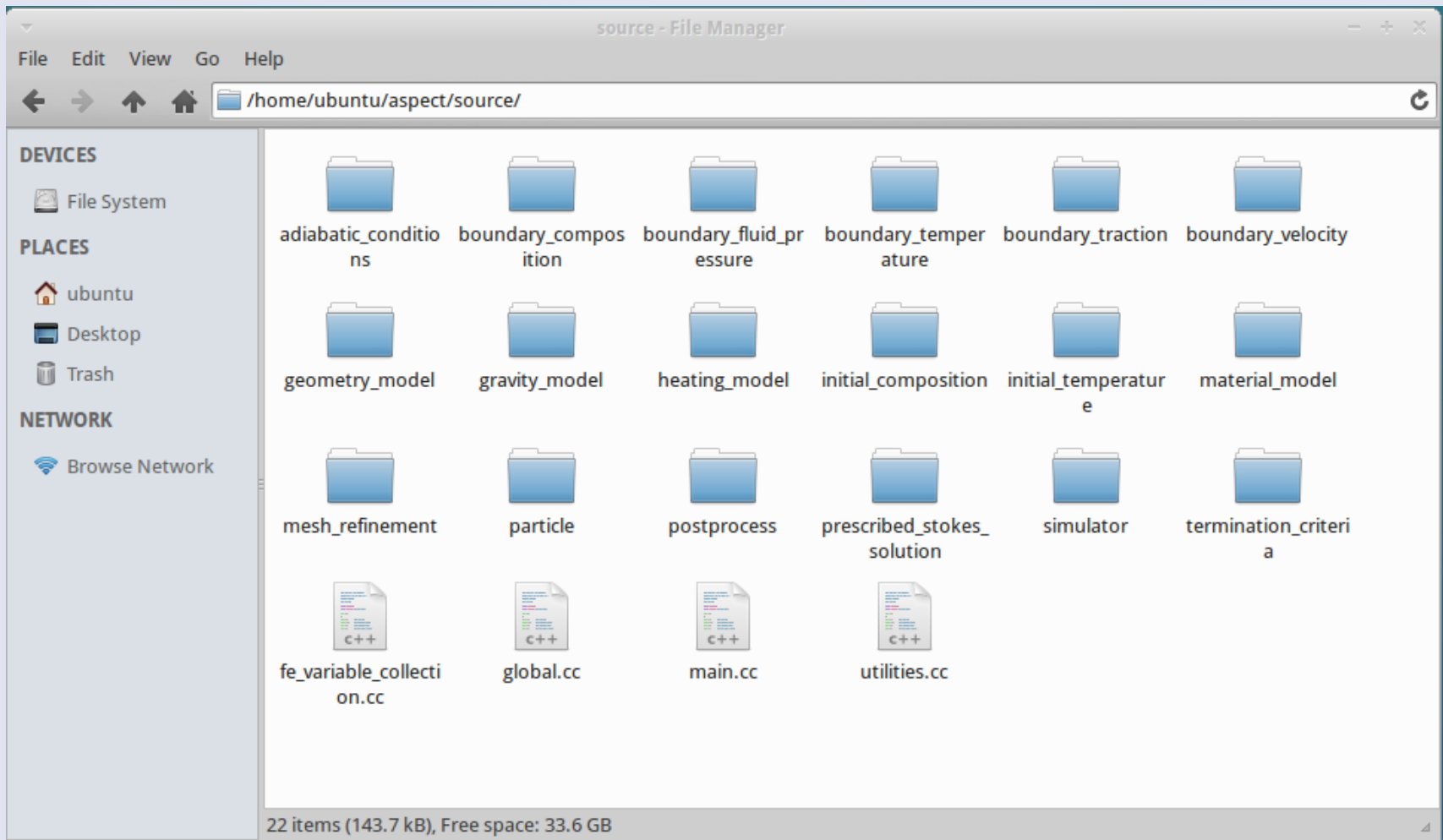
Modularity



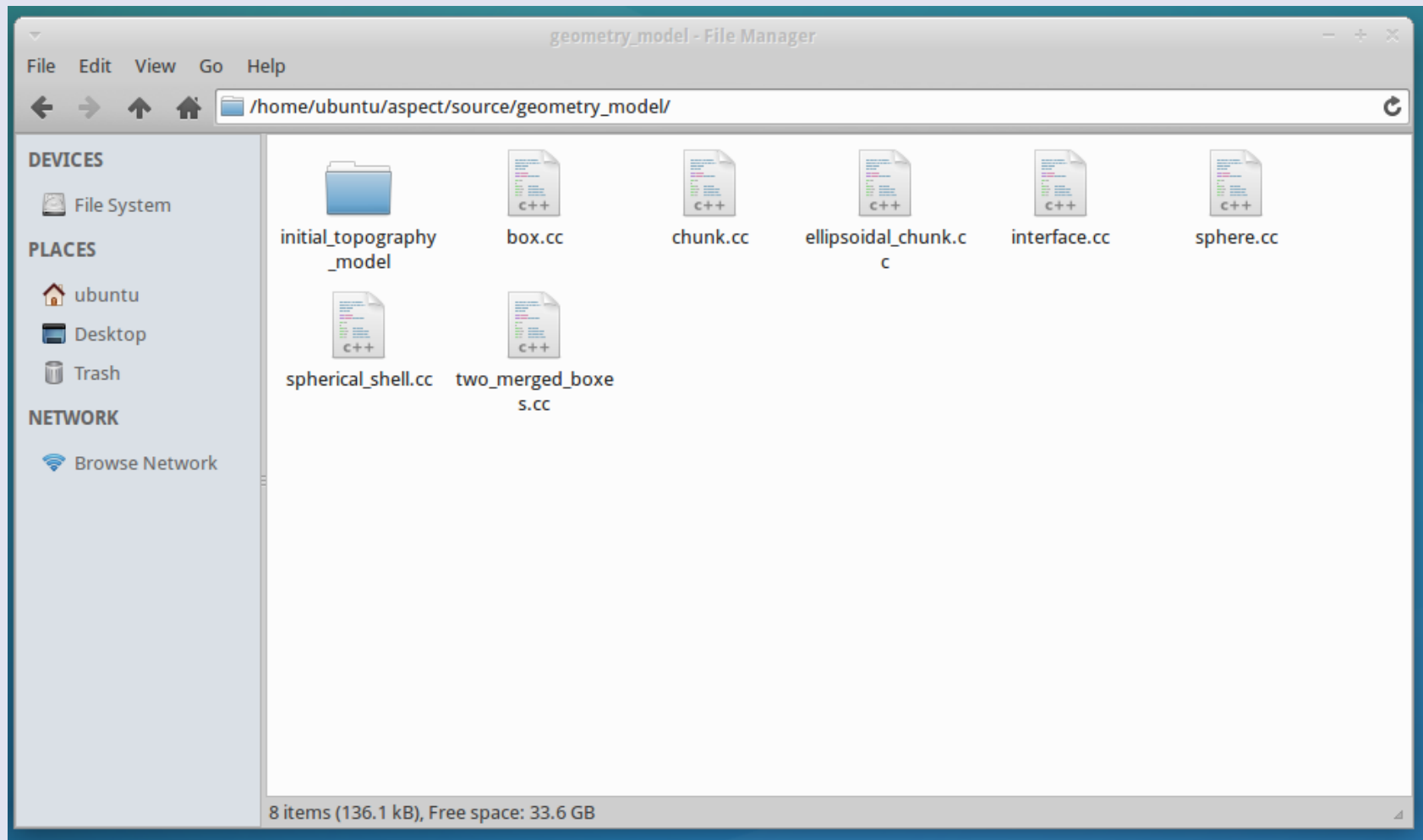
Modularity



Modularity



Modularity



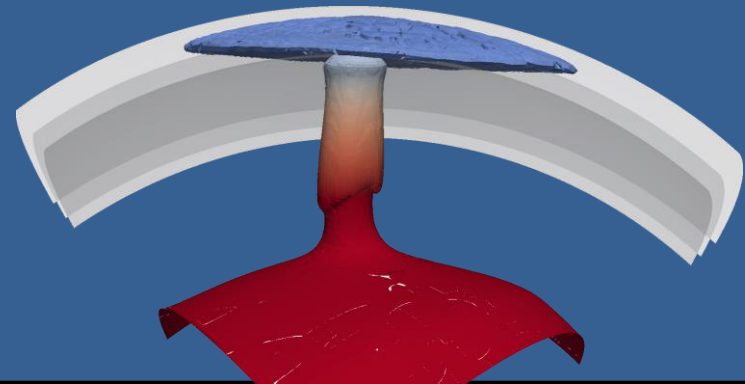
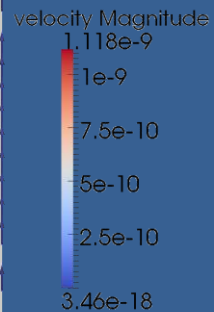
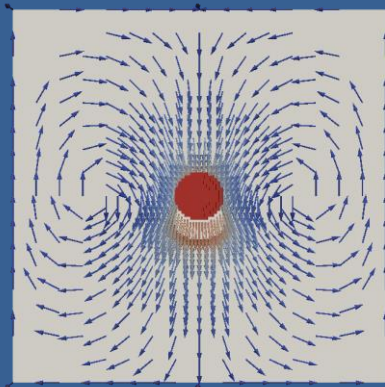
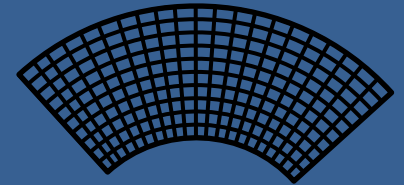
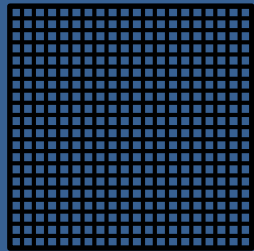
Geometry model

2D or 3D?

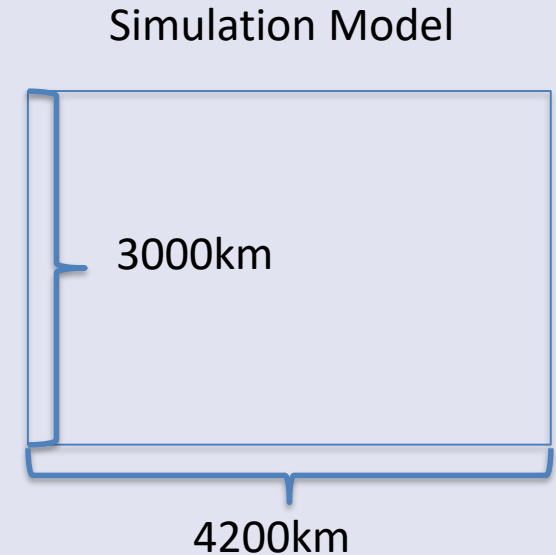
Geometry model

Box

Spherical shell



- Aspect has many built in geometry models such as “box” and “spherical shell”.
- A box is a rectangle in 2D and a cuboid in 3D.
- The width (X extent) of the box is 4.2×10^6 meters and the depth (Y extent) is 3×10^6 meters.
- The choice of meters as the unit of length is external to the parameter file; i.e. the user has to ensure the consistency of the various units used in the parameter file.



```
21 subsection Geometry model
22     set Model name = box
23     subsection Box
24         set X extent = 4.2e6
25         set Y extent = 3e6
26     end
27 end
```

```
subsection Geometry model
  set Model name = spherical shell

  subsection Spherical shell
    set Inner radius = 3481000
    set Outer radius = 6336000
    set Opening angle = 90
  end
end

subsection Gravity model
  set Model name = radial constant
end
```

The gravity model has to
be changed together with
the geometry

A peek into the code

- Take a look into:

`aspect/source/material_model/simpler.cc`

ASPECT General advice

Guidance for debug vs. optimized mode:

- ***Always*** test all new setups, models, and plugins in debug mode first
 - This makes finding bugs *much much simpler!*
- Run production runs with
 - more mesh refinement
 - optimized mode
- ***Never*** run production runs in debug mode – it is a waste of CPU time
(Remember: 1 CPU hour = \$0.10)

Dealing with errors

```
Terminal
File Edit View Terminal Tabs Help
-----
-- This is ASPECT, the Advanced Solver for Problems in Earth's ConvecTion.
--   . version 2.0.0-pre
--   . running in OPTIMIZED mode
--   . running with 1 MPI process
--   . using Trilinos
-----

Line <1> of file <input string>: No entry with name <Output diectory> was declared in the current subsection.

-----
Exception 'dealii::ExcMessage ("Invalid input parameter file.")' on rank 0 on processing:
-----
An error occurred in line <343> of file </home/ubuntu/aspect/source/main.cc> in function
void parse_parameters(const string&, dealii::ParameterHandler&)
The violated condition was:
false
Additional information:
Invalid input parameter file.
-----

Aborting!
-----
```

- The error message often already tells you what the problem is!

- To create an ASPECT executable in release mode type in a terminal:

```
mkdir ~/aspect/release  
cd ~/aspect/release  
cmake -DCMAKE_BUILD_TYPE=Release ~/aspect  
make -j2 (may take 30 min)
```
- To run release mode use:

```
~/aspect/release/aspect tutorial.prm
```
- Verify this by looking at the
 - first lines of output
 - timing information that is output every 100 time steps

ASPECT can run in parallel on a single machine:

- Multiple executables running at the same time on the same machine can communicate

- To try this:

```
mpirun -np 2 ./aspect tutorial.prm
```

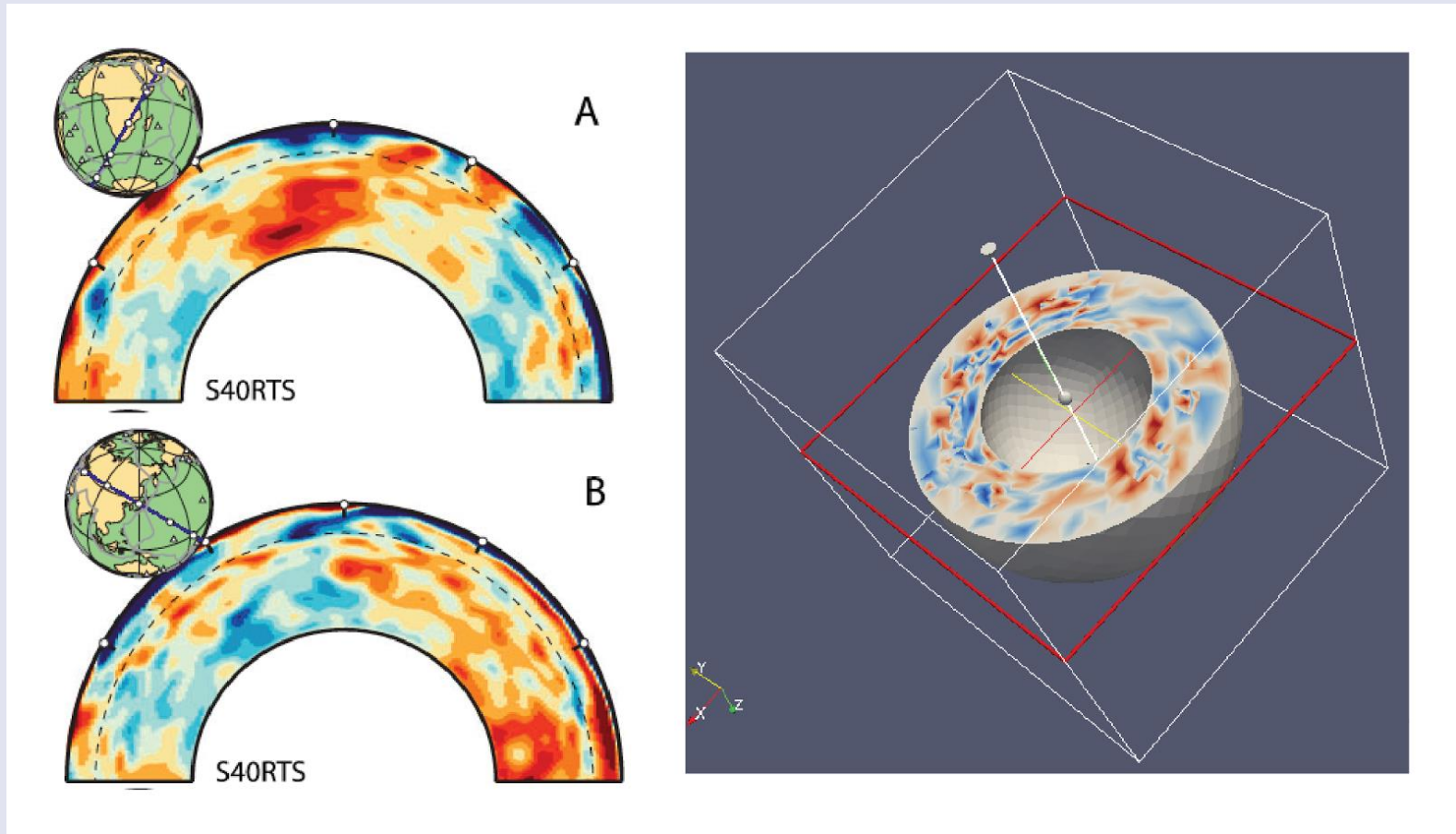
(“np” = “number of processes”)

- Verify this by looking at the
 - first lines of output
 - timing information that is output every 100 time steps

General guideline:

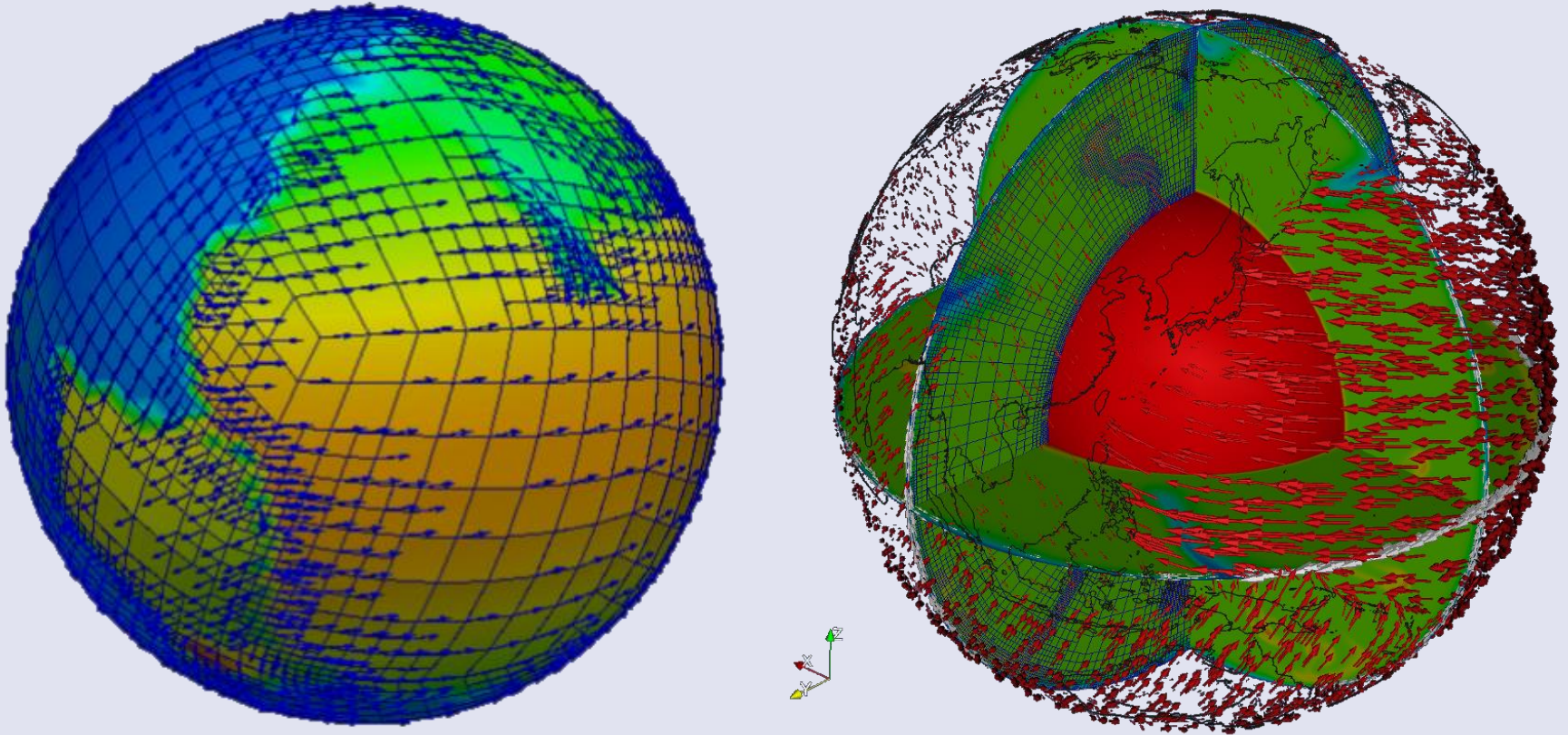
- Using more processors is faster if every processor has at least 30,000 degrees of freedom
 - find the number of freedom at the top of *log.txt*
- If you do have a large problem, use
 - as many processors as you have
 - but no more than $\#DoFs / 30,000$
- For example:
 - *tutorial.prm* with 3 global refinements has 948 DoFs
 - *tutorial.prm* with 5 global refinements has 13,764 DoFs
- Neither of these benefits much from parallelization: The cost of communication is larger than the gain due to parallelization!

- 5.3.4 3D convection with an Earth-like initial condition



From J. Austermann

- 5.3.5 Using reconstructed surface velocities by GPlates



From R. Gassmoeller

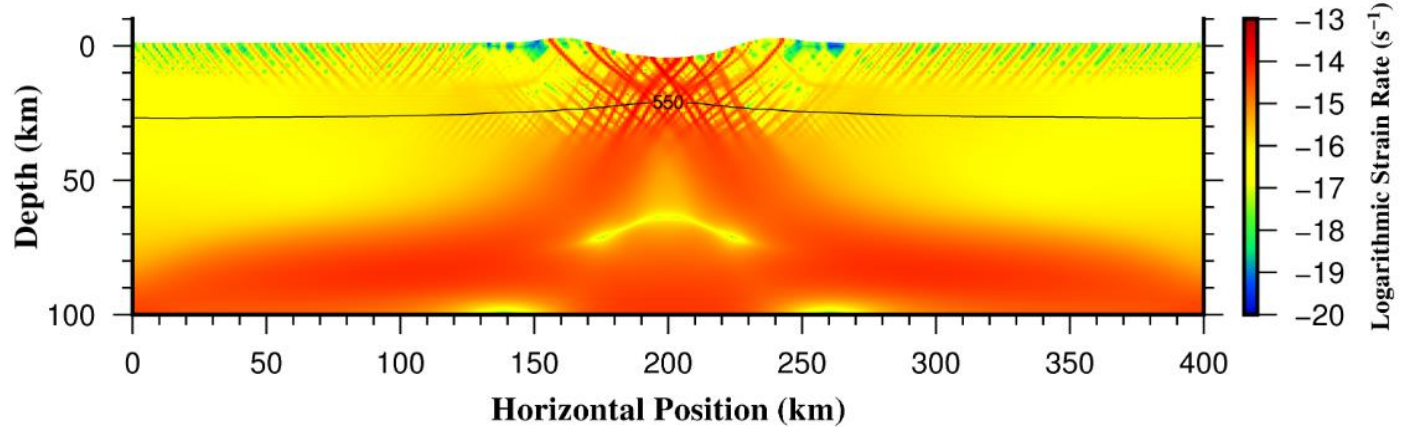
GPlates

- 5.3.11 Melt migration in a 2D mantle convection model



Time: 0.00e+00 years

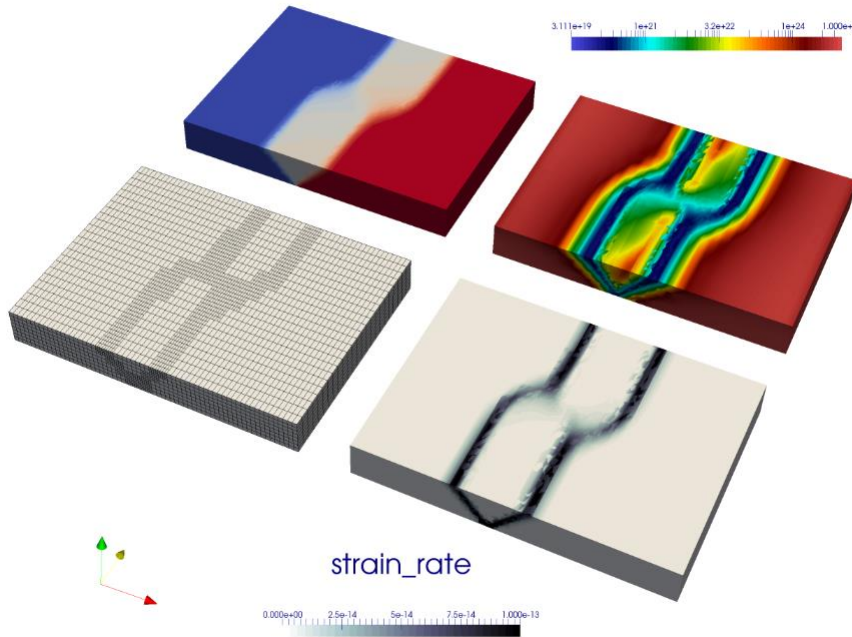
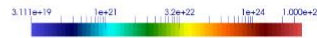




velocity X



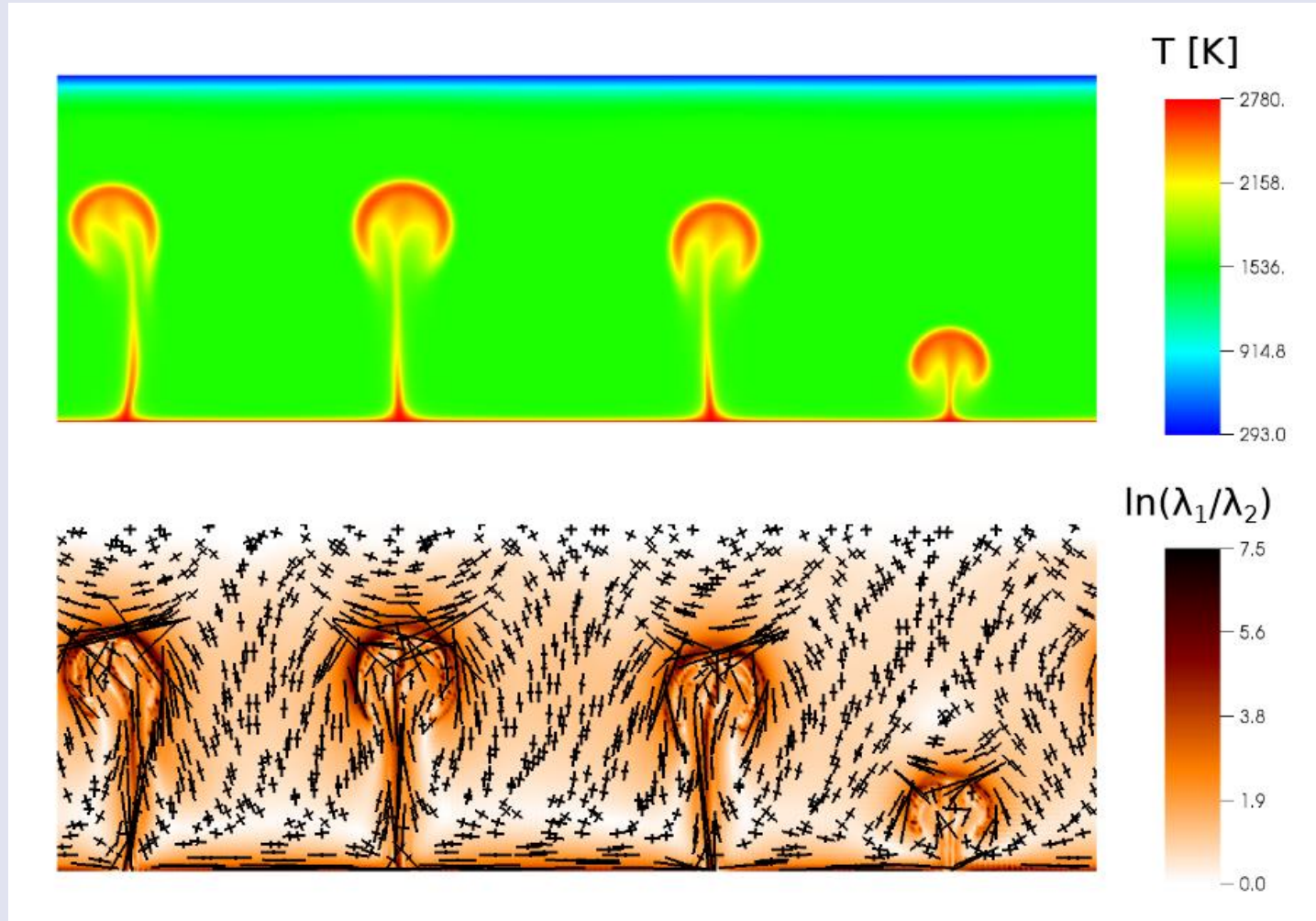
viscosity



- 5.3.8 Crustal deformation and 5.3.9 Crustal extension

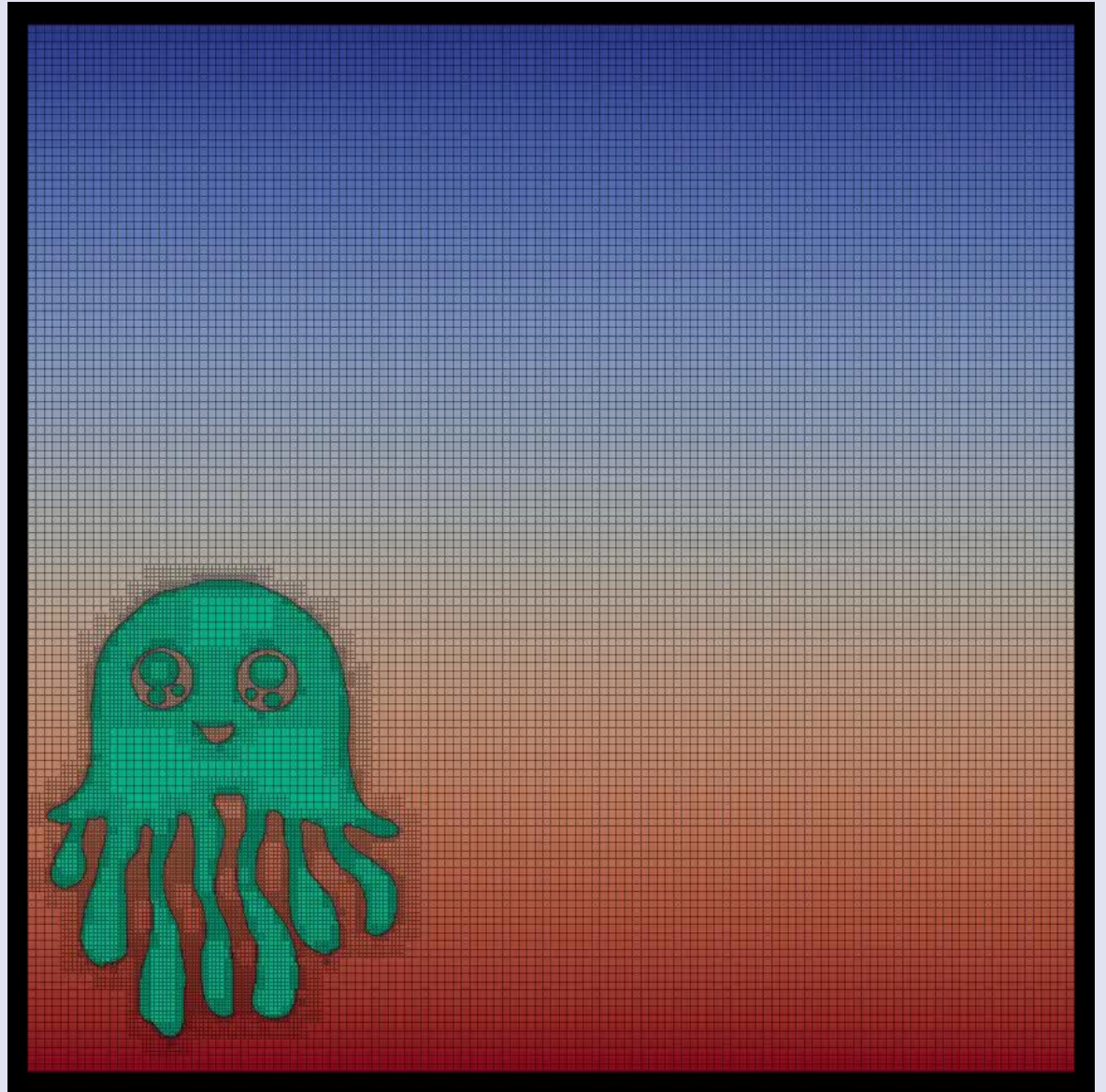
Tracking finite strain

- 5.2.11 Tracking finite strain

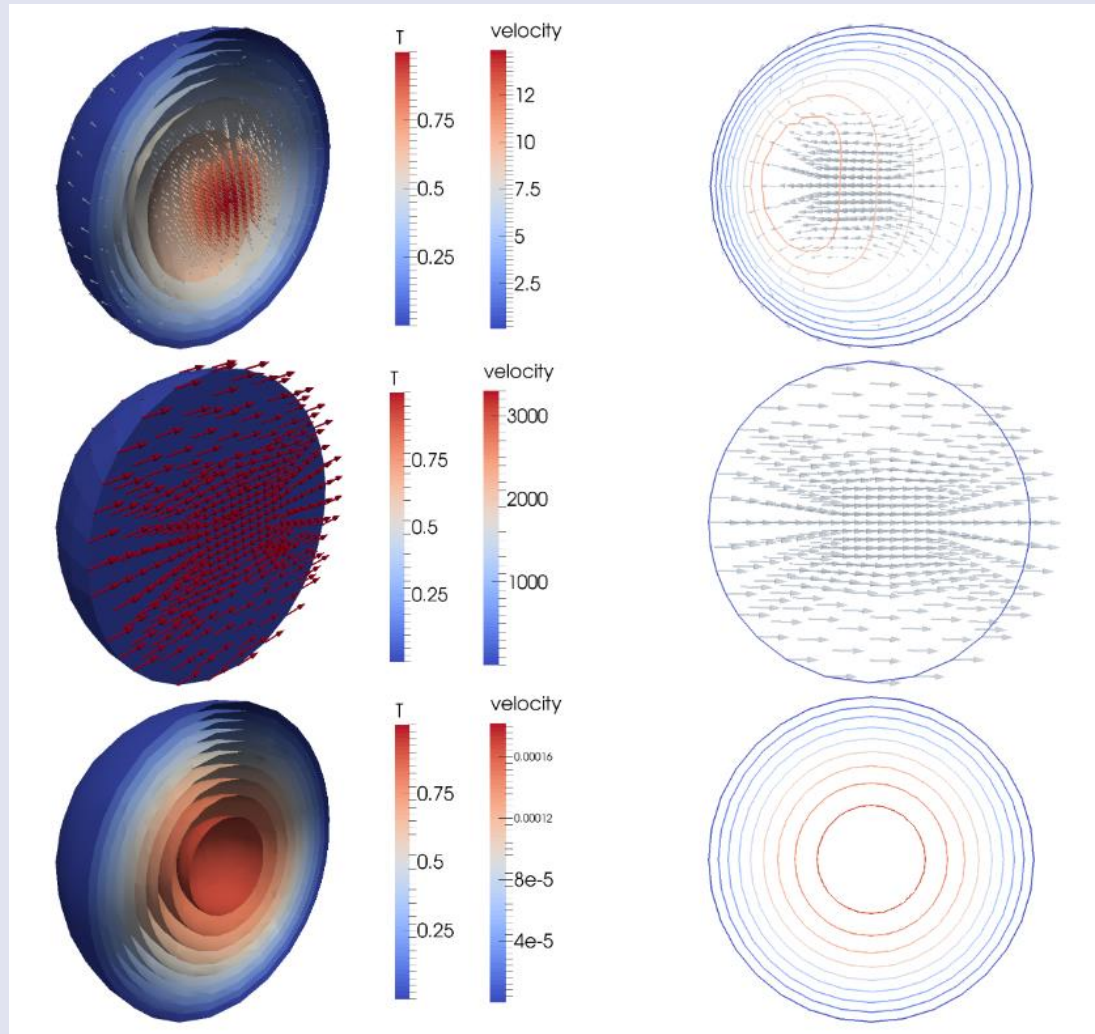


Convecting arbitrary shapes

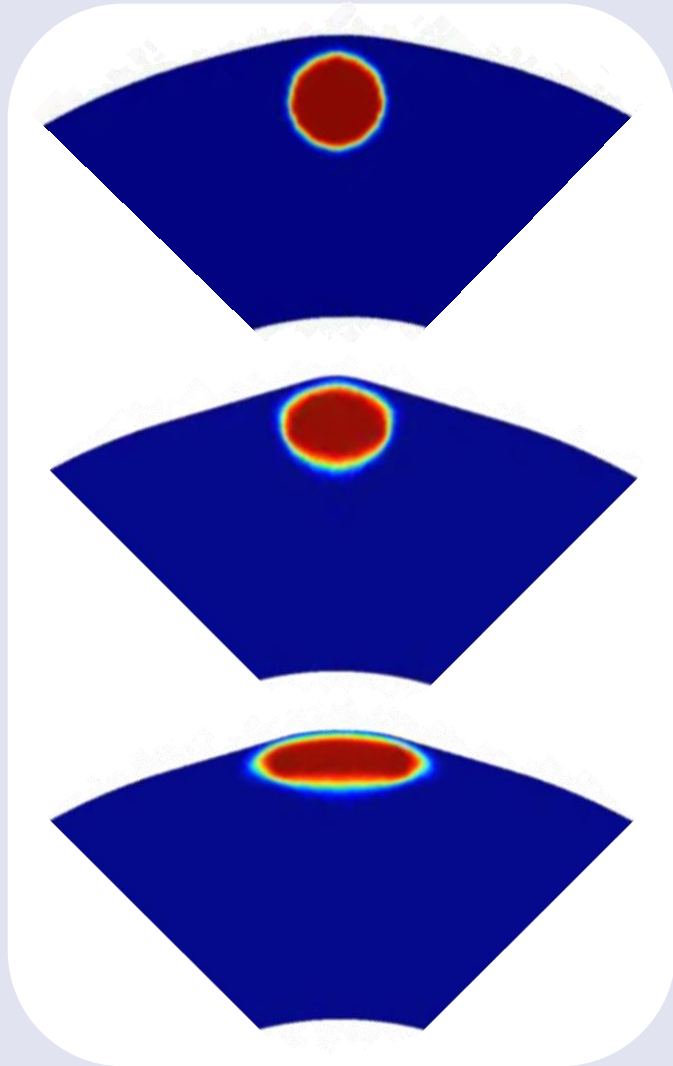
- 5.2.12 Reading in compositional initial composition files generated with geomIO



- 5.3.10 Inner core convection

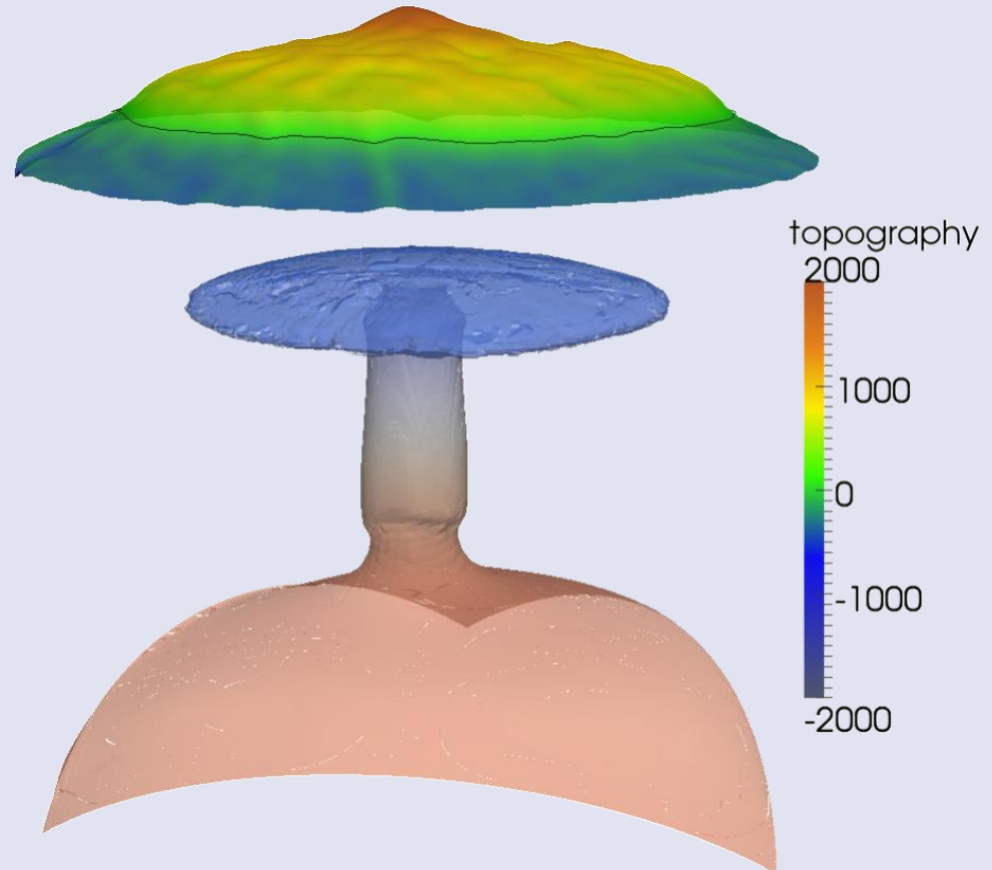


Surface topography

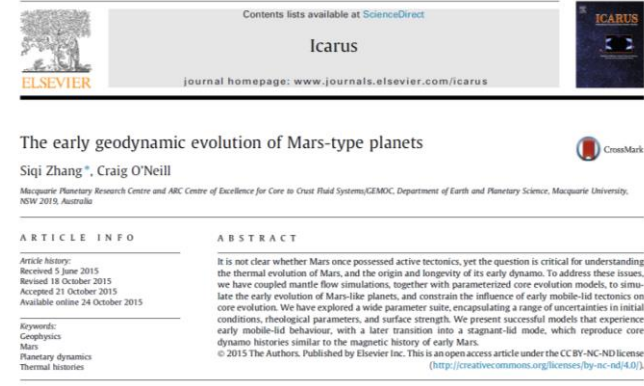
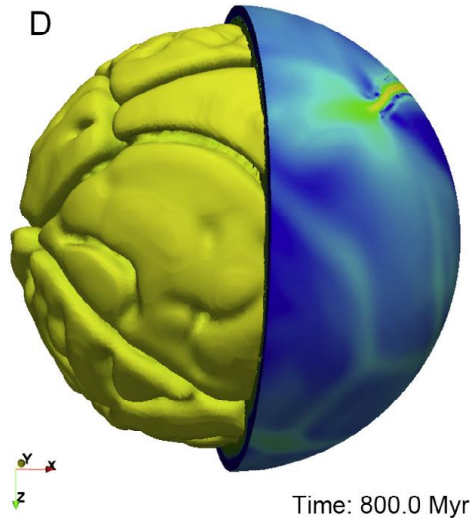
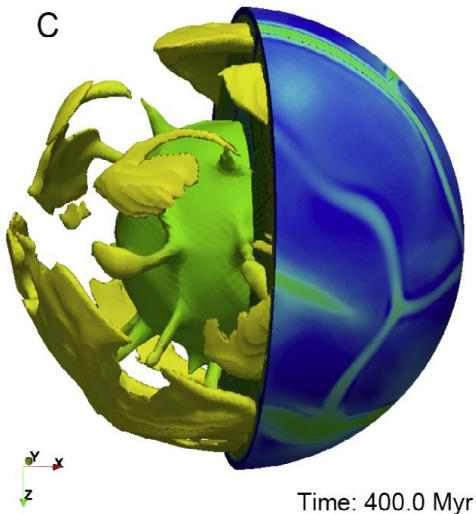
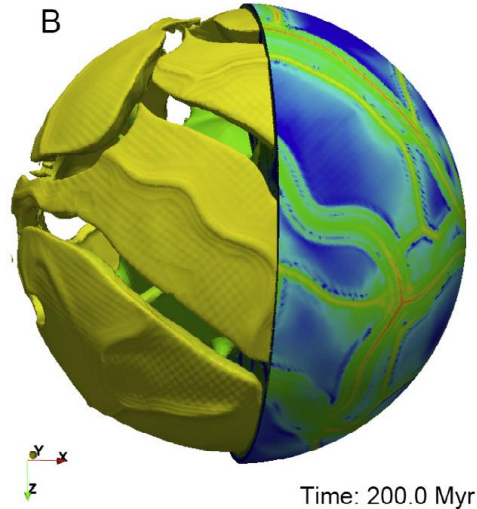
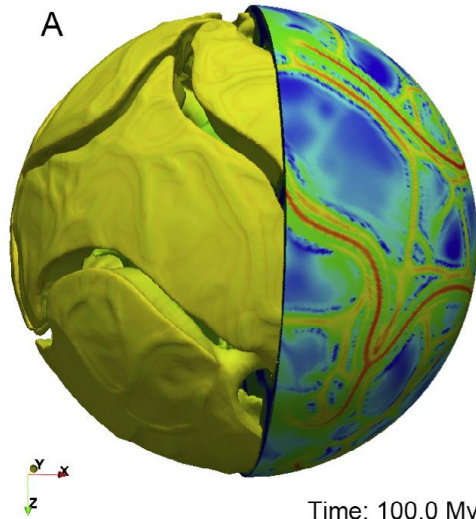


From I. Rose

- 5.2.6 Using a free surface and
- 5.2.7 Using a free surface in a model with a crust

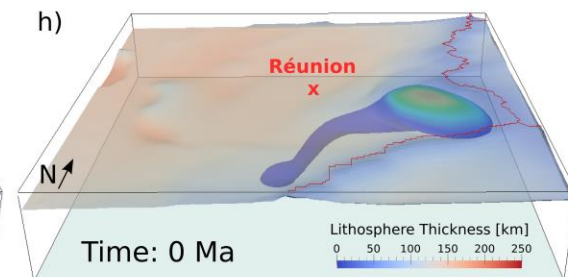
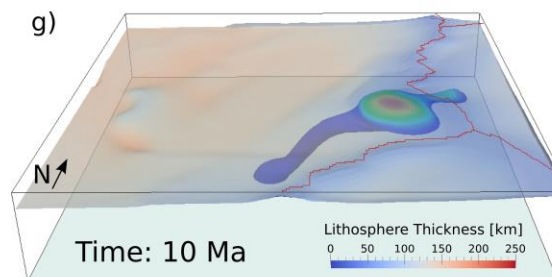
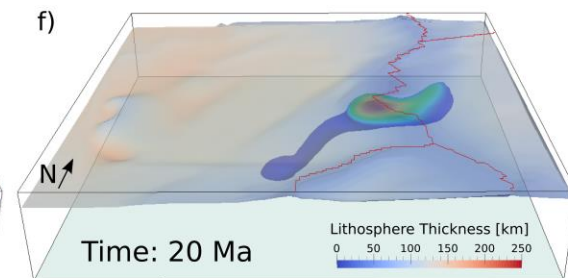
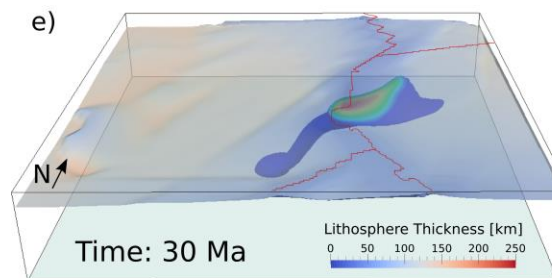
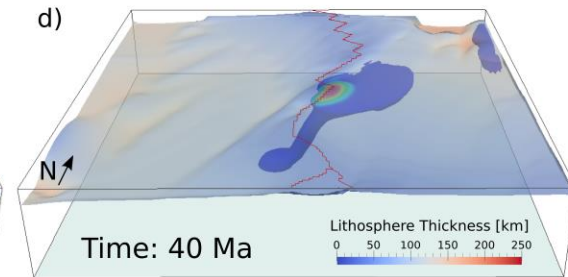
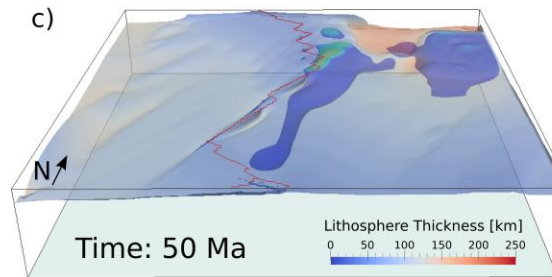
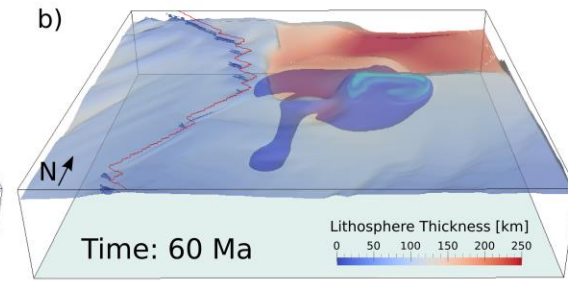
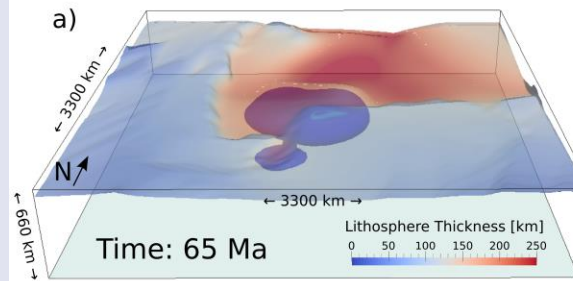
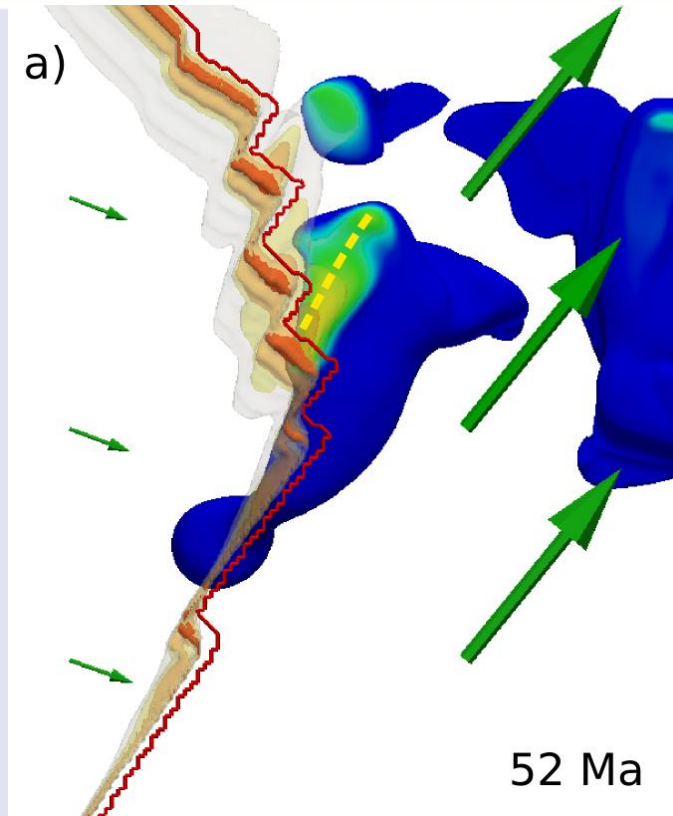


Evolution of Mars



Siqi Zhang, Craig O'Neill,
**The early geodynamic
evolution of Mars-type
planets, In Icarus,
Volume 265, 2016,
Pages 187-208.**

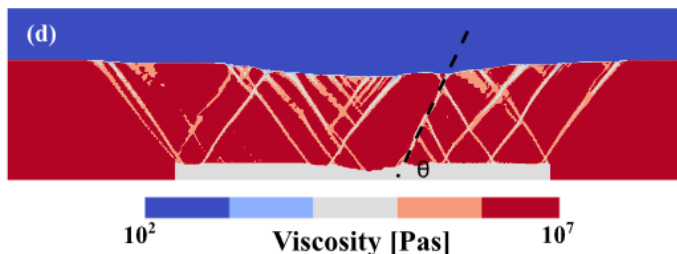
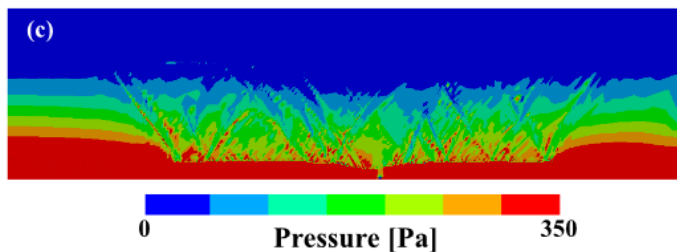
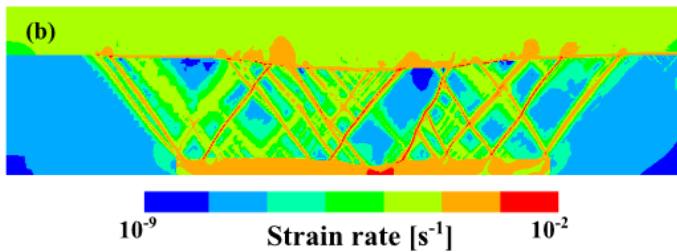
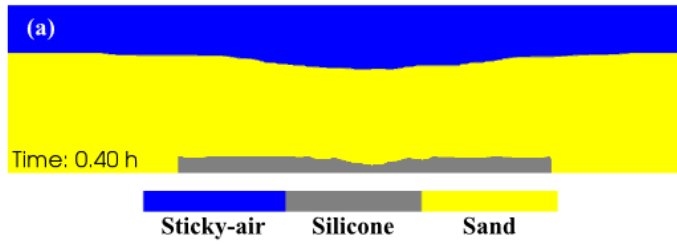
Plume-ridge interaction



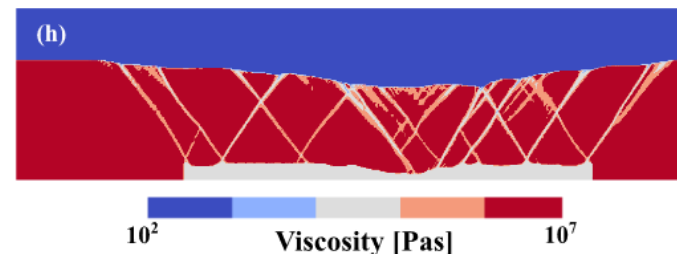
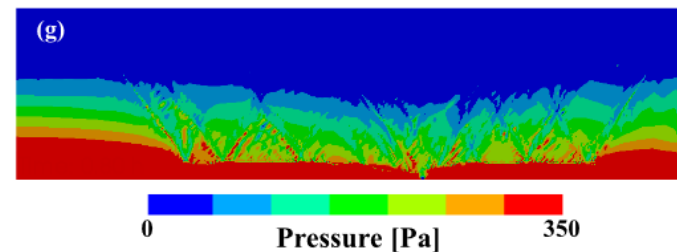
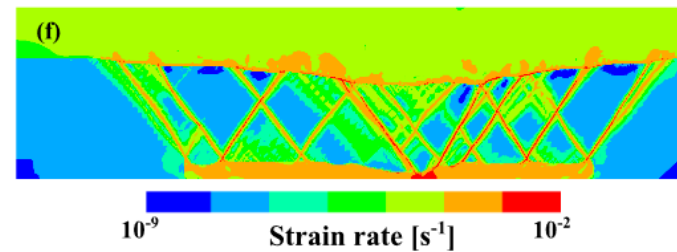
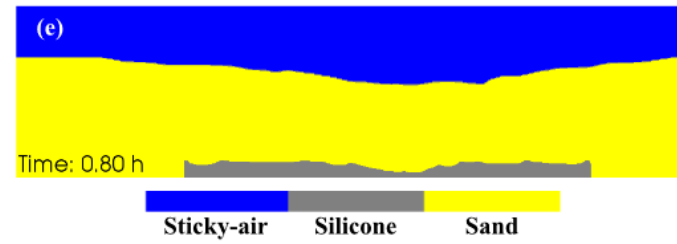
Eva Bredow, Bernhard Steinberger, Rene Gassmöller, Juliane Dannberg,
How plume-ridge interaction shapes the crustal thickness pattern of the Réunion hotspot track. *Geochemistry, Geophysics, Geosystems* 18(8), 2930–2948.

Deformation of the crust

0.994 cm of extension

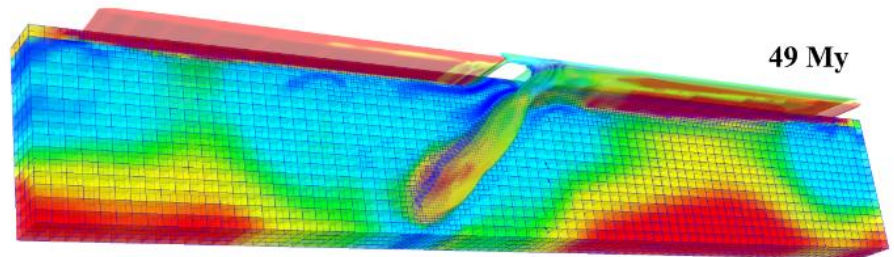
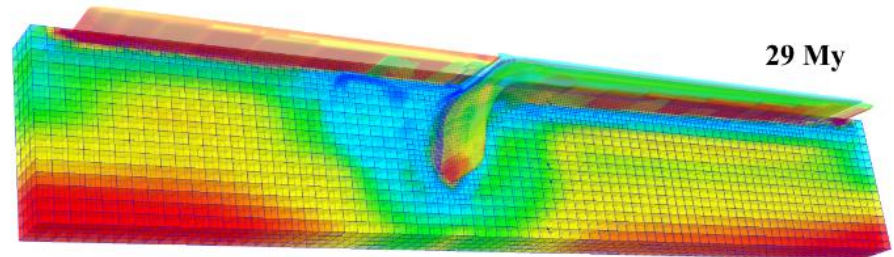
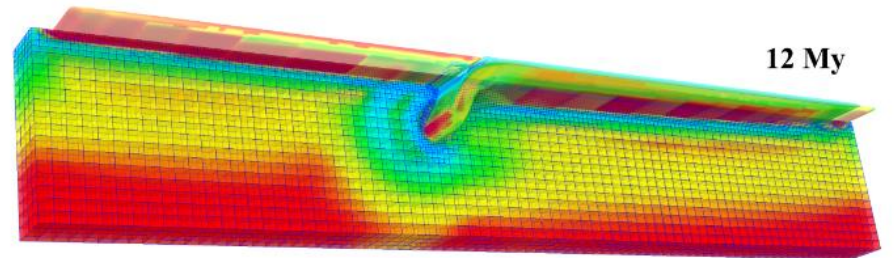
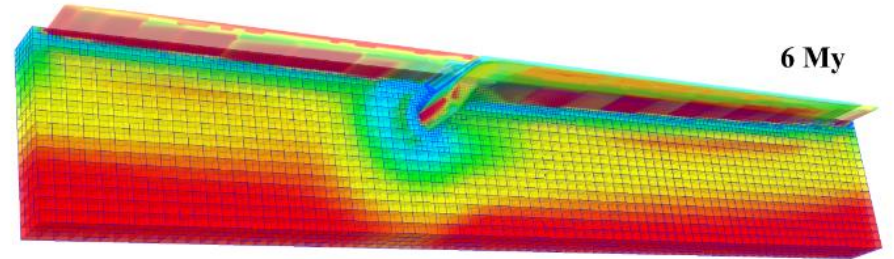
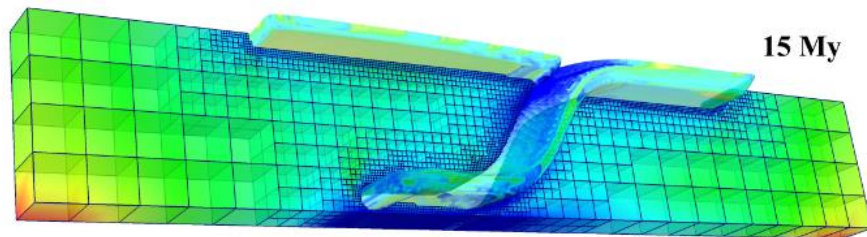
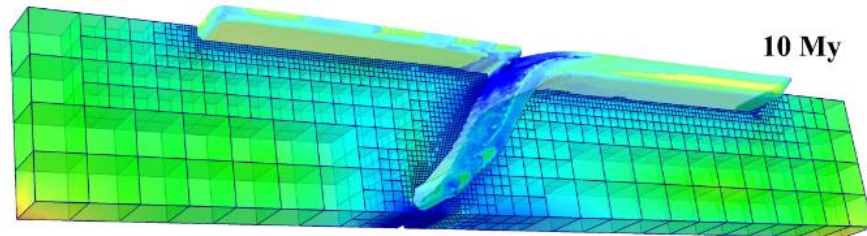
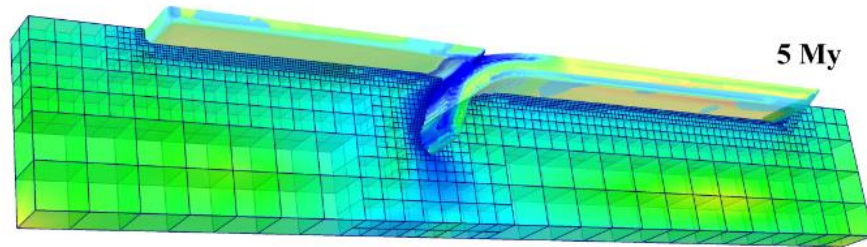
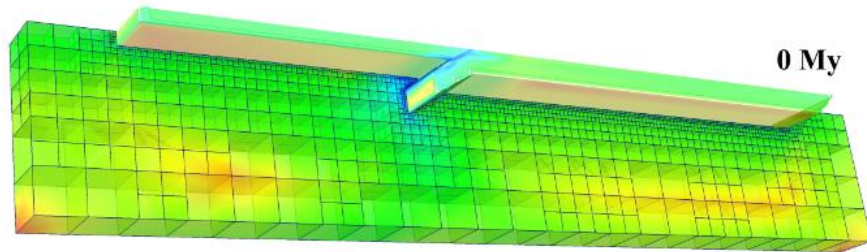


1.989 cm of extension

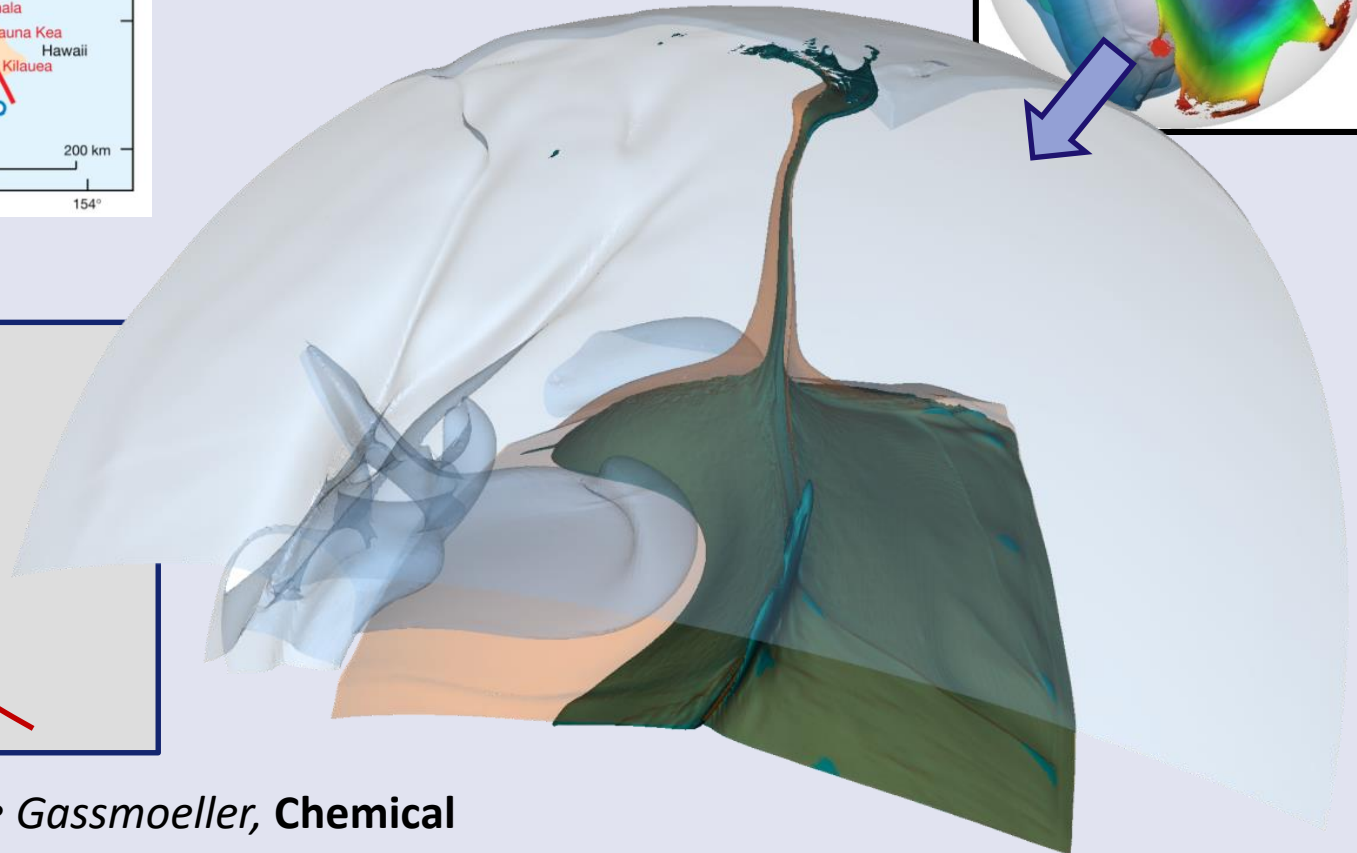
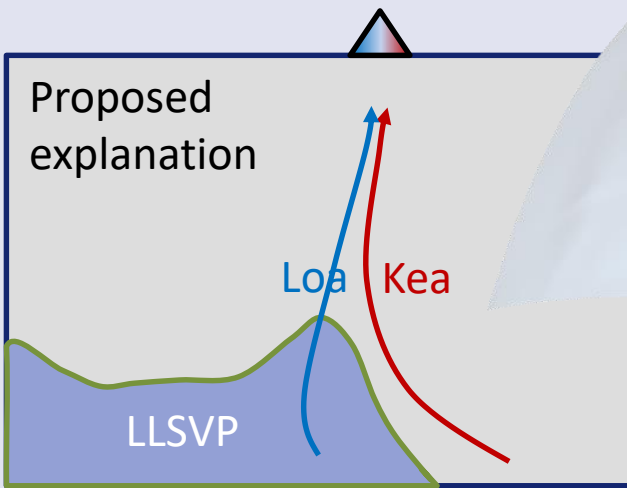
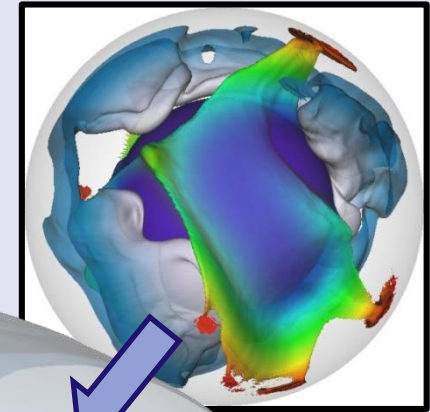
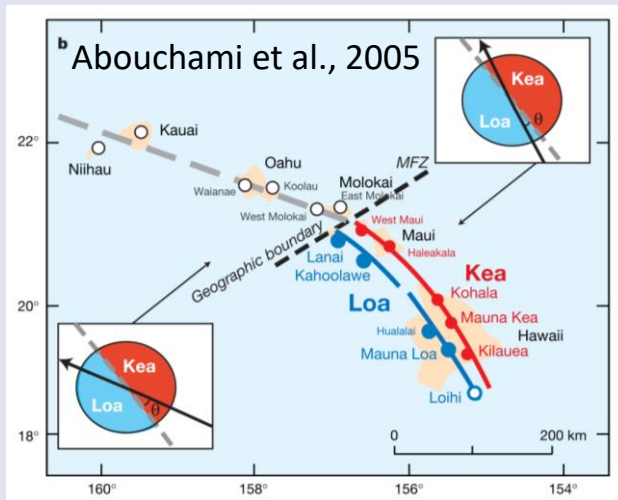


Glerum, A., Thieulot, C., Fraters, M., Blom, C., and Spakman, W.: Implementing nonlinear viscoplasticity in ASPECT: benchmarking and applications to 3D subduction modeling, Solid Earth Discuss., <https://doi.org/10.5194/se-2017-9>, in review, 2017.

How does subduction work?



Asymmetry of mantle plumes



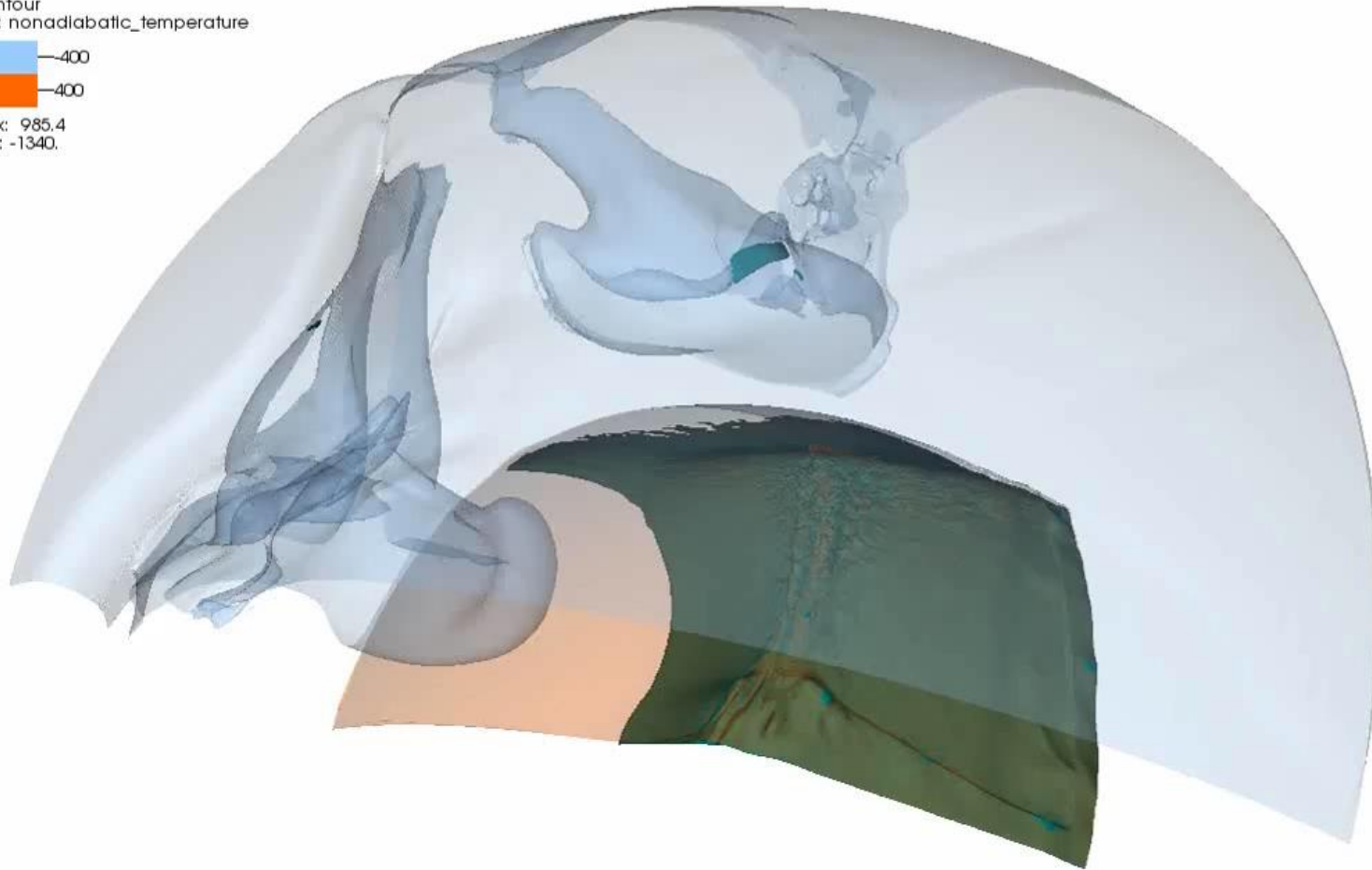
Juliane Dannberg, Rene Gassmoeller, Chemical trends in ocean islands explained by plume--slab interaction, PNAS, 2018.



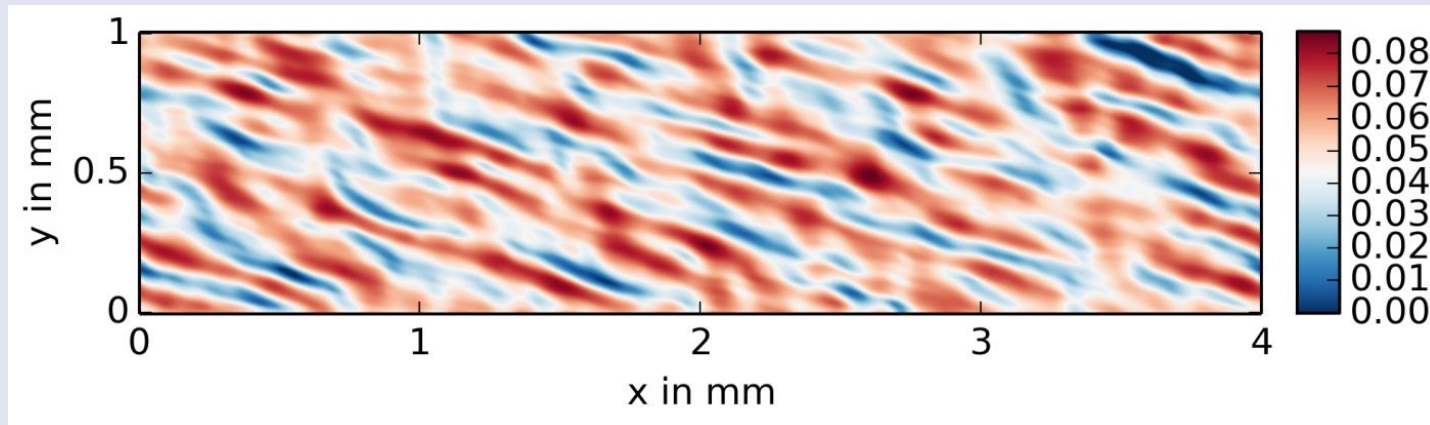
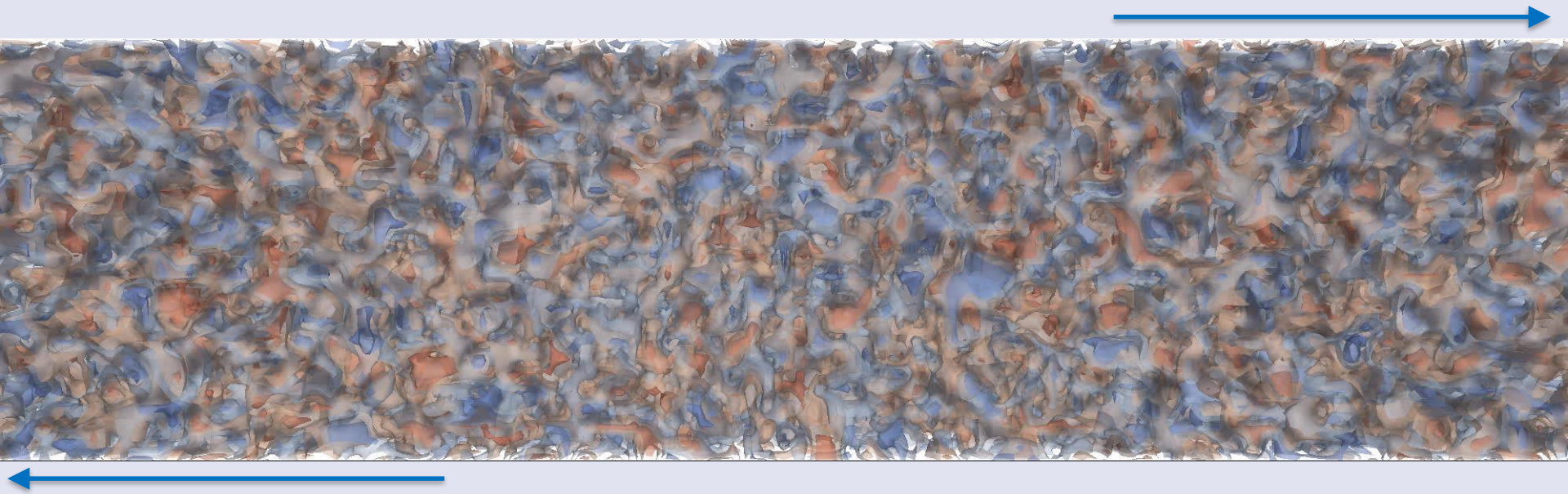
Time = 0...250 Ma

Contour
Var: MORB
0.4200
Max: 1.009
Min: 0.007082

Contour
Var: nonadiabatic_temperature
400
400
Max: 985.4
Min: -1340.



Deforming melt & solid rocks

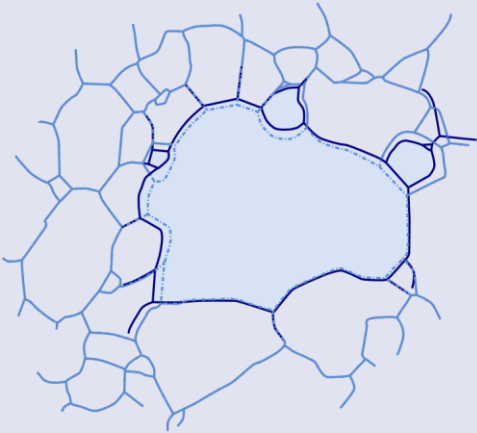


J. Dannberg, T. Heister (2016). **Compressible magma/mantle dynamics: 3-D, adaptive simulations in ASPECT**, Geophysical Journal International., Vol. 207(3), pp. 1343-1366.

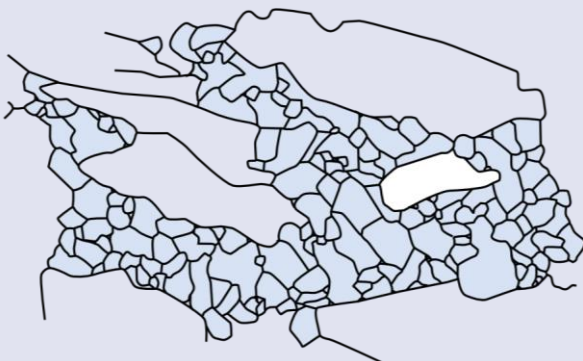
Effects of grain size on convection

Deformation

Grain growth:
Ripening by diffusion

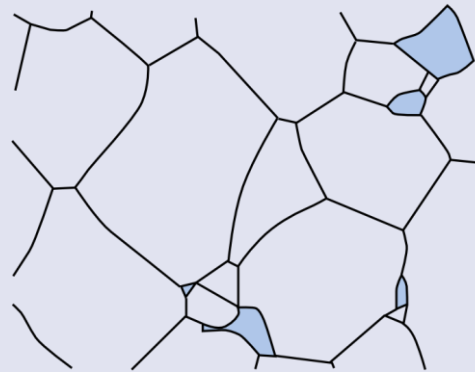


Grain size reduction:
Dynamic recrystallisation

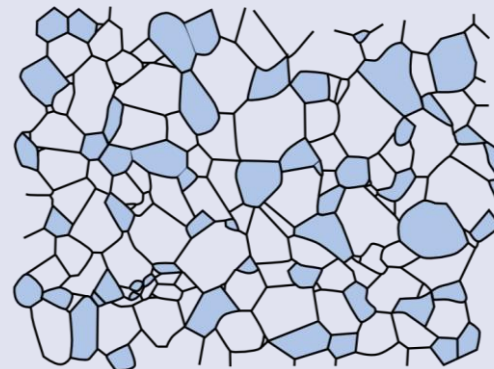


Pinning

One mineral dominates:
Rapid growth

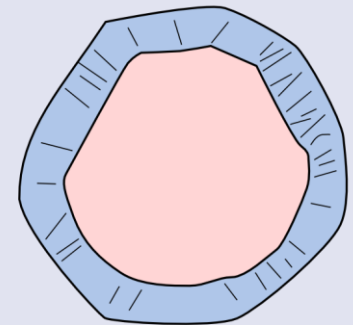


Similar volume fractions:
Slow growth

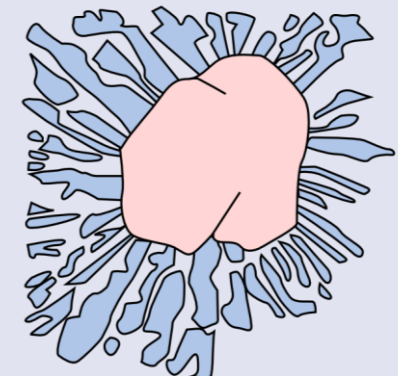


Reaction

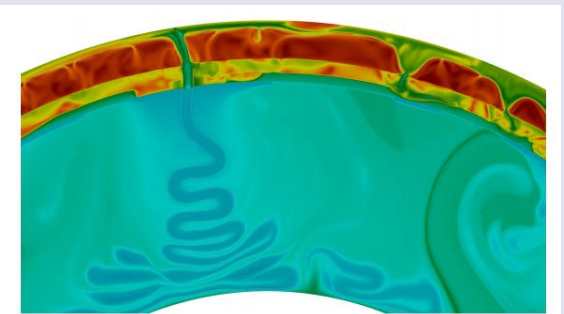
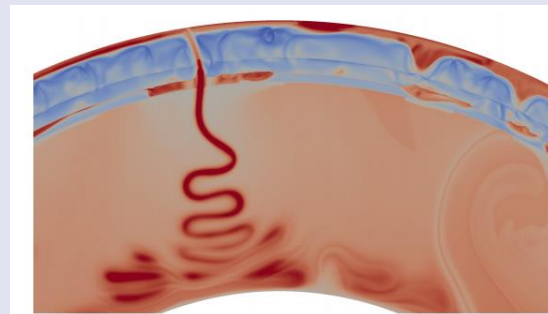
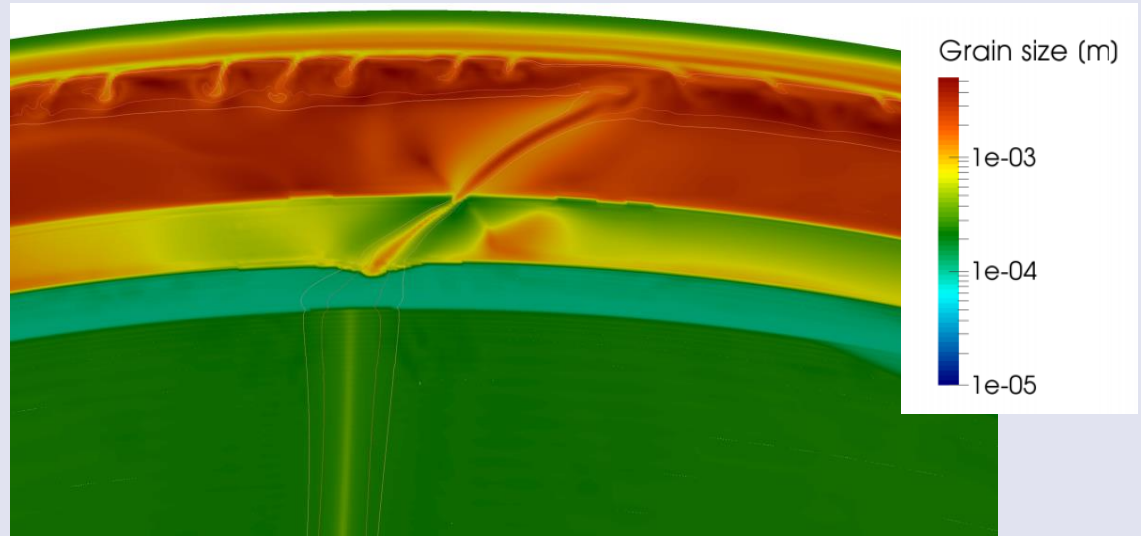
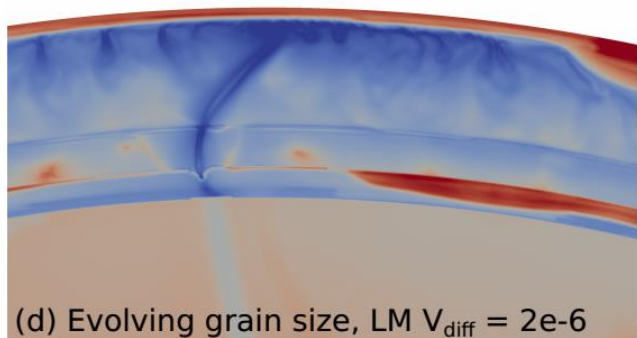
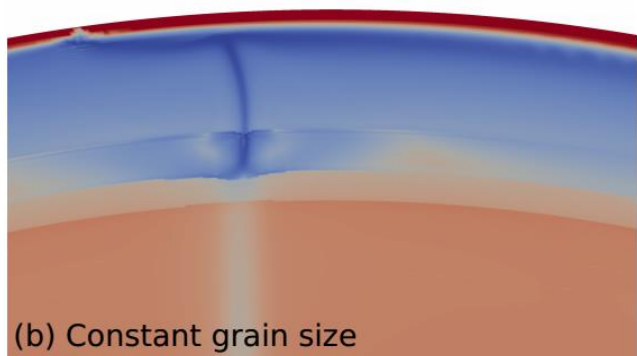
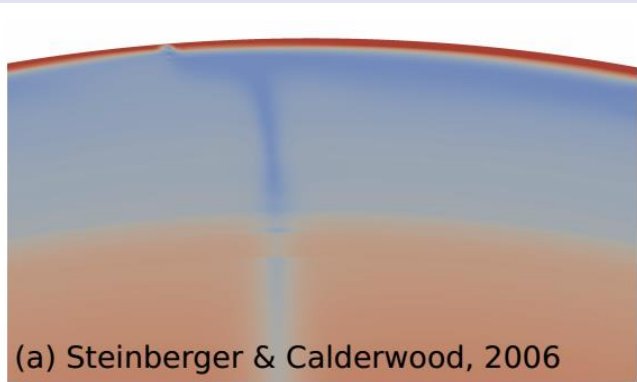
Polymorphism:
Coherent nucleation



Decomposition:
Symplectite formation



Effects of grain size on convection



J. Dannberg, Z. Eilon, U. Faul, R. Gassmüller, P. Moulik, R. Myhill (2017). The importance of grain size to mantle dynamics and seismological observations. Geochemistry, Geophysics, Geosystems 18 (8), 3034–3061.