Tutorial IV
Multi-material, self-consistent subduction with a free surface[1]

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[1]Schmeling et al., PEPI, 2008

GeoMod2014

Recap Tutorial III

Succeeded in:

- Setting up a model with one compositional heterogeneity
- Using ASPECT's function parser
- Setting up mesh-independent initial conditions
- Tackling benchmark problems

Goals Tutorial IV

By the end of this tutorial, you should be able to

- Write and install new material **plugins**
- Modify the input parameter file for a **subduction** model with multiple materials
- Understand issues regarding **averaging**
- Understand the concept of "**sticky-air**" and its effect on the solver

Simple subduction

Start simple:

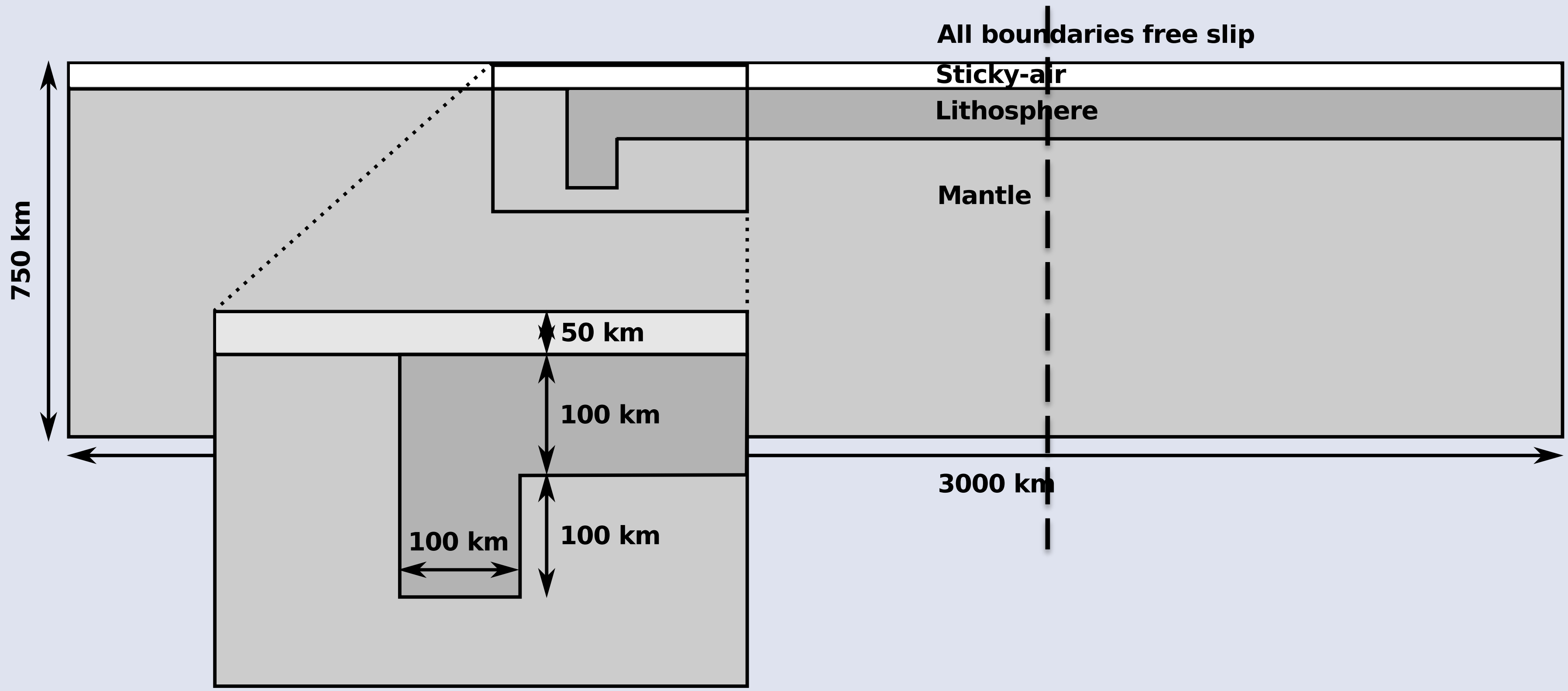
Subduction model of

Schmeling et al. 2008 (PEPI 171)

- 2D
- No temperature effects
- Constant viscosities
- Benchmark →

  results of other codes to compare

Schmeling et al. 2008 subduction



Schmeling et al. 2008 subduction

Although a relatively simple setup,

it discusses very important points:

- Effect of different **averaging** methods on viscosities near rheological boundaries
- **Decoupling** subducting plate from the surface
- Approximation of **free surface** through sticky-air

Sticky-air

- Thin layer of relatively low viscosity (10^{19} Pas) and density (0 kg/m^3) to allow for surface deformation
- No need to deform grid, but
- High viscosity contrasts and
- High resolution needed

Tasks

Changes compared to Tutorial III:

- Prescribe parameters of multiple (>2) materials
- Implement 4 different types of averaging of materials

→

1. Modify schmeling_empty.prm
2. Write a new Material Model based on assigned averaging method
3. Run simulation and visualize results
4. Report slap tip depth after 1 and 2 My

Editing the input file

We will begin by editing the input file

1. Change to the appropriate directory

```
> cd ~/ASPECT_TUTORIAL/models
```

2. Open the parameter file for editing

```
> gedit schmeling_empty.prm
```

Editing the input file

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Now read through the following sections in the input file and edit the red sections:

1. Global parameters
2. Geometry model
3. Compositional fields
4. Material model
5. Compositional initial conditions

Editing the input file

Global parameters

```
set Dimension                                   = 2
set Start time                                  = 0
set End time                                    = 0
set Use years in output instead of seconds = true
set Number of cheap solver steps               = 0
set Output directory                            = schmeling
```

Geometry model

```
subsection Geometry model
  set Model name = box
  subsection Box
    set X extent = 2000000
    set Y extent = 750000
    set X repetitions = 3
  end
end
```

Editing the input file

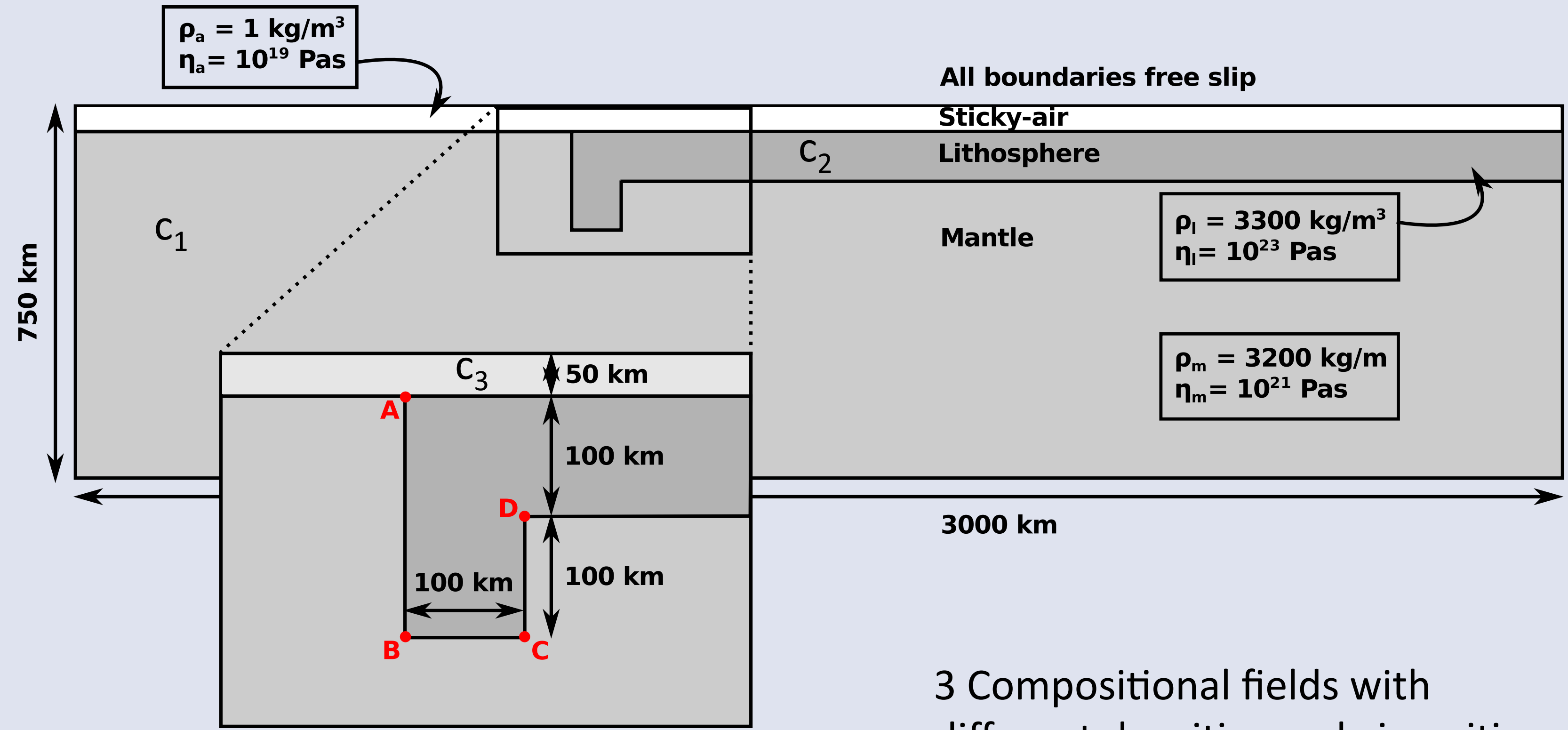
Compositional fields

```
subsection Compositional fields
  set Number of fields          =
end
subsection Compositional initial conditions
  set Model name                = function
  subsection Function
    set Variable names          = x, z
    set Function constants     = Ax = 1000000.0, Az=700000.0, Bz=500000.0,
                                  Cx=1100000.0, Dz=600000.0
    set Function expression    = \
                 if((z<Bz)|(x<Ax&z<Az)|(x>Cx&z<Dz),1,0); \ #mantle
                 if((x>=Ax&z>=Dz&z<Az)|(x>=Ax&x<=Cx&z>=Bz&z<Dz),1,0); \ #lithosphere
                 if(z>=Az,1,0) # air
  end
end
```

How many compositional fields? For simplicity, we describe all materials as fields

You already know how to use the function parser!

Editing the input file



3 Compositional fields with different densities and viscosities

Editing the input file

Material model

```
subsection Material model
  set Model name = XXX
  subsection XXX model
    set Thermal conductivity              = 0.0
    set Thermal expansion coefficient     = 0.0
    set Reference specific heat           = 1.0
    set List of densities of fields       =
    set List of viscosities of fields     =
  end
end
```

Normally, here you provide a functional name for your new Material Model plugin

No temperature effects

Here we provide the densities and viscosities of the compositions to the Material Model plugin. Use the same order as in the definition of the compositional fields.

Material Model plugins

1. Change to the appropriate directory

   > cd ~/ASPECT_TUTORIAL/aspect/source/material_model

2. What files are there?

   interface.cc

   simple.cc

   simpler.cc

   steinberger.cc

   table.cc …

   Material Model plugins

Plugin organization

Plugins:

- for Geometry, Material, Gravity etc. in ~/source
- derive from interface.cc
- can be selected from the input file

A Material Model plugin should at least provide

1. Viscosity
2. Density
3. Specific heat
4. Thermal conduct.
5. Thermal expansion
6. Compressibility

The Material Model plugin – viscosity function

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So far, we used Material Model simple.cc

```
> gedit simple.cc
```

```
template <int dim>
double
Simple<dim>::
viscosity (const double temperature,
           const double pressure,
           const std::vector<double> &composition,
           const SymmetricTensor<2,dim> &strain_rate,
           const Point<dim> &position) const
```

The Material Model plugin – viscosity function

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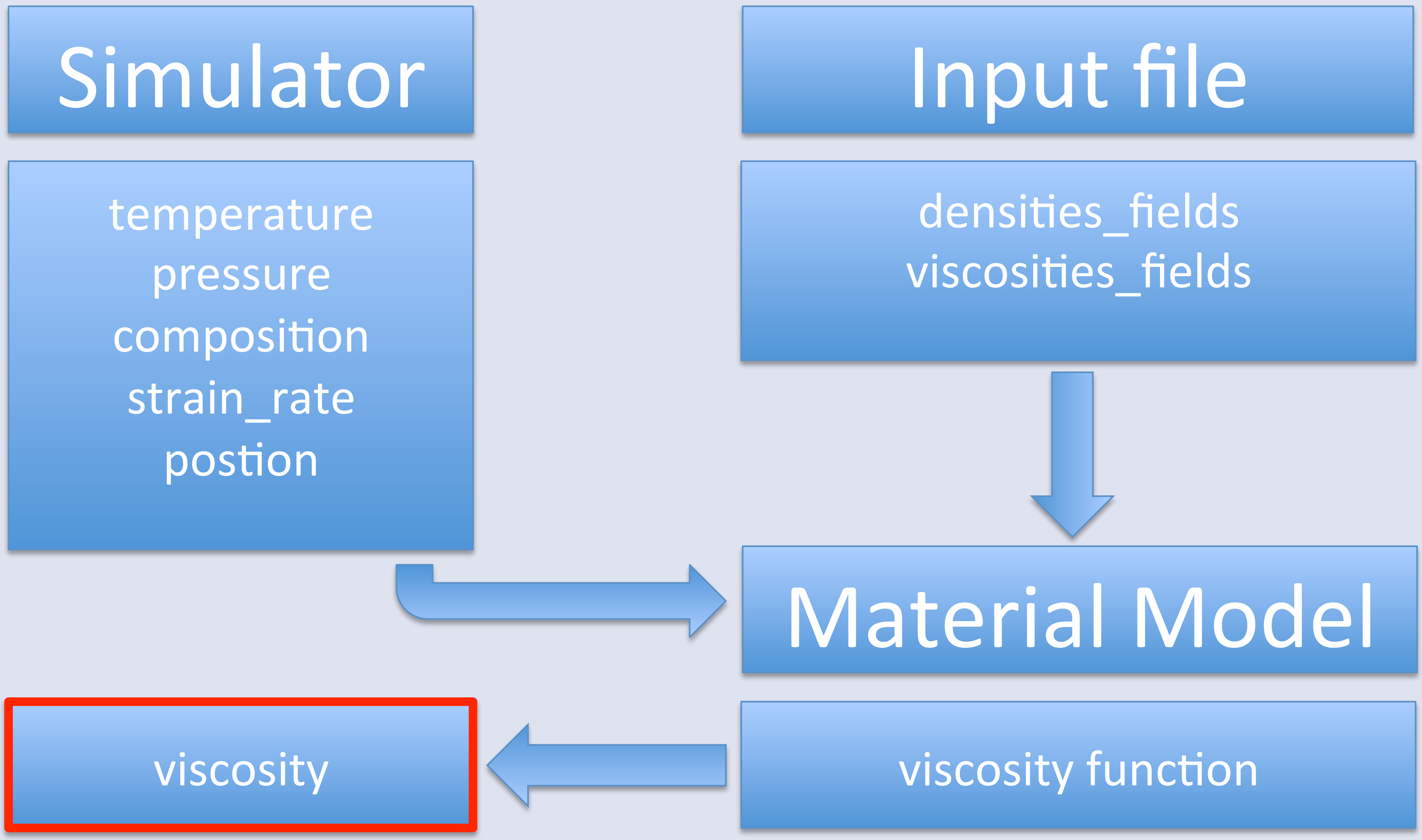

The Material Model plugin – viscosity function

So far, we used Material Model simple.cc

```
> gedit simple.cc
```

```
const double delta_temp = temperature-reference_T;
const double temperature_dependence = (reference_T > 0
            ? std::max(std::min(std::exp(-thermal_viscosity_exponent*delta_temp/
reference_T),1e2),1e-2)
            : 1.0);
 double composition_dependence = 1.0;
 if ((composition_viscosity_prefactor != 1.0) && (composition.size() > 0))
   { return (pow(10, ((1-composition[0]) * log10(eta*temperature_dependence)
                        + composition[0] * log10(eta*composition_viscosity_prefactor
                                                  *temperature_dependence))));
   }
 return composition_dependence * temperature_dependence * eta;
```

The Material Model plugin – viscosity function

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

So far, we used Material Model simple.cc

```
> gedit simple.cc
```

```
if (composition.size() > 0)
   { return (pow(10, ((1-composition[0]) * log10(eta)
                                         + composition[0]  * log10(eta*composition_viscosity_prefactor));
   }
```

What kind of averaging?

Writing a viscosity function

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ASPECT: build on others!

→

- XXX.cc is a slightly adapted copy of simple.cc
- Implement a viscosity function (line 35) that averages the contribution of the fields as follows:
  - Group 1: Harmonic averaging
  - Group 2: Geometric averaging
  - Group 3: Arithmetic averaging
  - Group 4: Infinite norm

Writing a viscosity function

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Group 1 - Harmonic

$$\eta_{harm} = \frac{c_1 + c_2 + c_3}{\frac{c_1}{\eta_1} + \frac{c_2}{\eta_2} + \frac{c_3}{\eta_3}}$$

Group 2 - Geometric

$$\log \eta_{geom} = \frac{c_1 \log \eta_1 + c_2 \log \eta_2 + c_3 \log \eta_3}{c_1 + c_2 + c_3}$$

Group 3 - Arithmetic

$$\eta_{arith} = \frac{c_1\eta_1 + c_2\eta_2 + c_3\eta_3}{c_1 + c_2 + c_3}$$

Group 4 - Infinite norm

$$\eta_{\inf} = \eta_{\max_i (c_i)}$$

Where c_i represent the values of the 3 compositional fields, and η_i are the viscosities of each corresponding field.

~/ASPECT_TUTORIAL/aspect/source/material_model/schmeling.cc is a working material model with each averaging method implemented in case you need it

Advection of a field

The advection of compositional fields can result in under- and overshooting of the c_i values near steep gradients →

1. *Prevent oscillations*

Stabilization (Guermond et al., J. Comput. Phys., 2011):

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

2. *Deal with oscillations*

Cut off c_i between 0 and 1

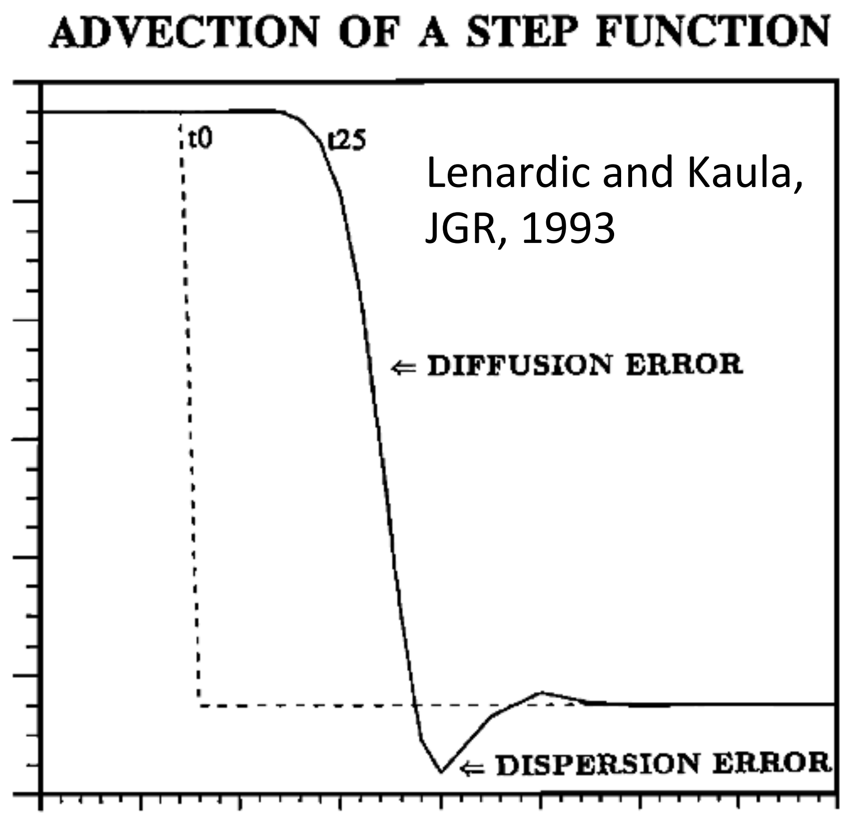

Fig. 1. Numerical advection of a step function over 25 Courant-Friedrichs-Lewy time steps. T0 is the initial step function and T25 is the advected step function. Two types of numerical errors are present: (1) numerical diffusion reflected in the tilting of the step; and (2) numerical dispersion resulting in the leading edge ripples. The numerical scheme employed was second-order accurate for smooth flow problems.

C++ syntax

- Always end declarations and assignments with ";"
- The first entry of a vector is accessed with "0":

  e.g. composition[0]
- Calculating a minimum of two numbers with:

  e.g. std::min(composition[0],1.0)

Plugin installation

```
> cd ~/ASPECT_TUTORIAL/aspect/include/  \
  aspect/material_model/
```

Here the corresponding header file XXX.h is located

```
> cd ~/ASPECT_TUTORIAL/aspect/debug
```

Normally, you would call

```
> cmake .
> make
```

Here we built the debug version, as opposed to the optimized release version

to compile and install your new plugin. Build system *cmake* will automatically detect it. Now you only need to call

```
> make -j2
```

Using ASPECT

Now run ASPECT in the terminal

1. Change to the appropriate directory

```
> cd ~/ASPECT_TUTORIAL/models/
```

2. Run ASPECT with the tutorial parameter file

```
> mpirun –np 2 aspect-debug schmeling_empty.prm
```

3. If correct,

```
> cd ~/ASPECT_TUTORIAL/aspect/release
> make –j2
```

4. Change model time to 2.5 My and rerun (this will take about 15 minutes, have a coffee)
5. Use ParaView to visualize slab evolution

```
> paraview schmeling/solution.pvd
```

Subduction evolution

Report slab tip depth after 1 and 2 My and model time

	Harmonic	Geometric	Arithmetic	Infinite
1 My Slab tip depth	(???)	(???)	(???)	(???)
2 My Slab tip depth	(???)	(???)	(???)	(???)
Model time after 15 min wall time	(???)	(???)	(???)	(???)

Subduction evolution

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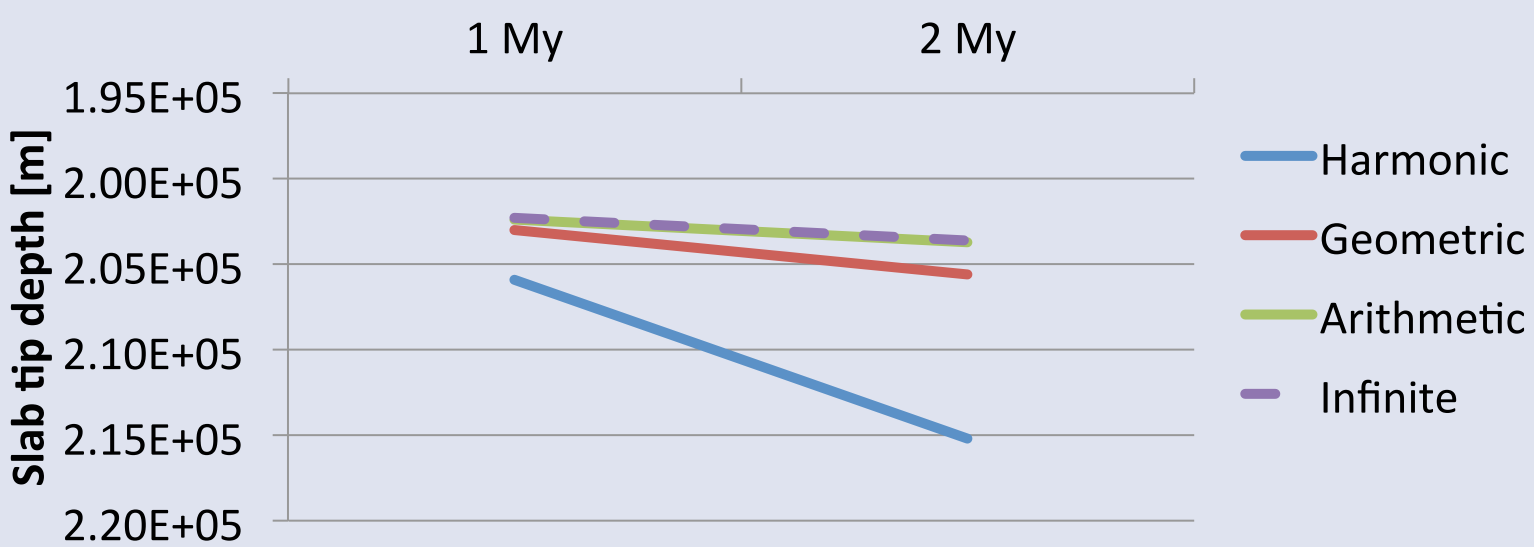
Finding slab tip depth in ParaView:
- Plot isocontour $C_2 = 0.5$

1. Use grid lines to estimate, or
2. Use Spreadsheet view of isocontour with
   Show only selected elements and
   3D view *Select Points On*, or
3. Use Spreadsheet view and Python calculator, or
4. Next time, write an ASPECT postprocessor ☺

Subduction evolution answer key

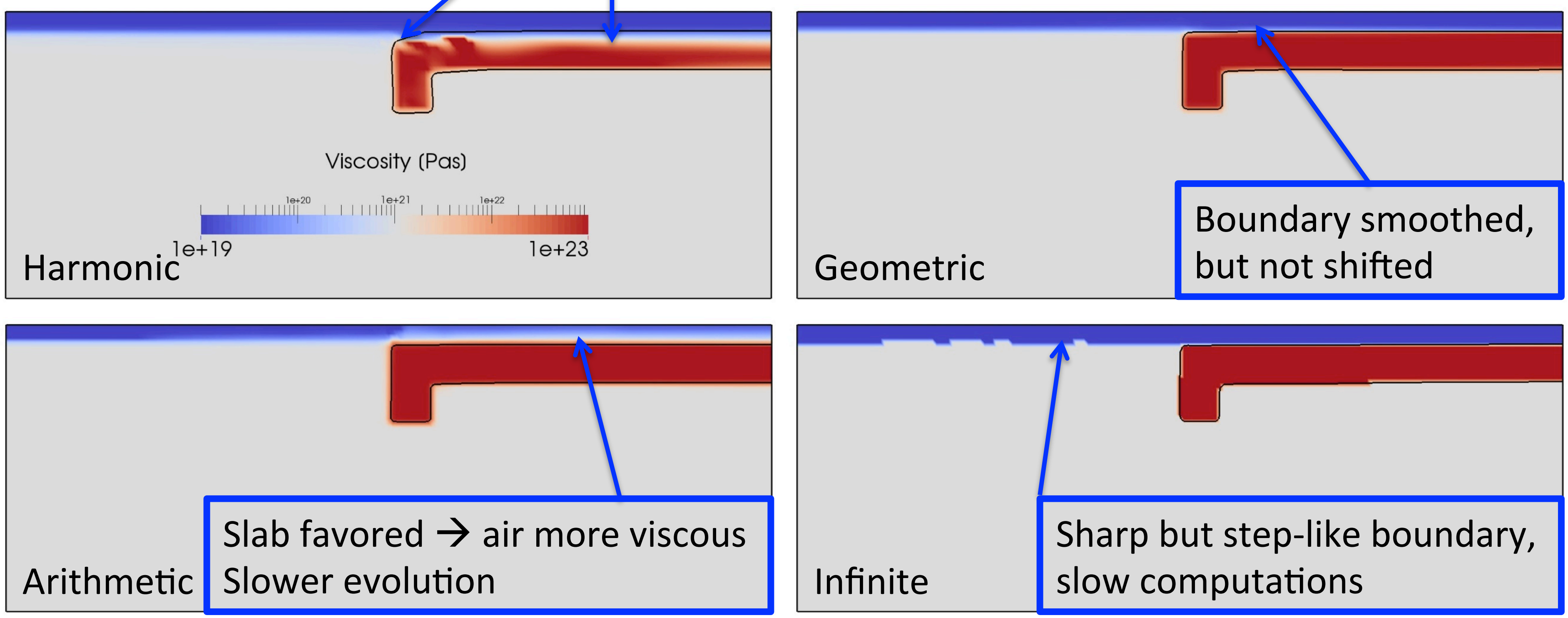
	Harmonic	Geometric	Arithmetic	Infinite
1 My Slab tip depth	205,892 m	202,983	202,387	202,291
2 My Slab tip depth	215,181 m	205,587	203,725	203,629
Model time after 15 min wall time	2.11903e6 yr	2.14136e6	2.20938e6	329,512



Results after 2 My

Slab detaching from surface

Air favored → slab thinned



So what averaging do we use?

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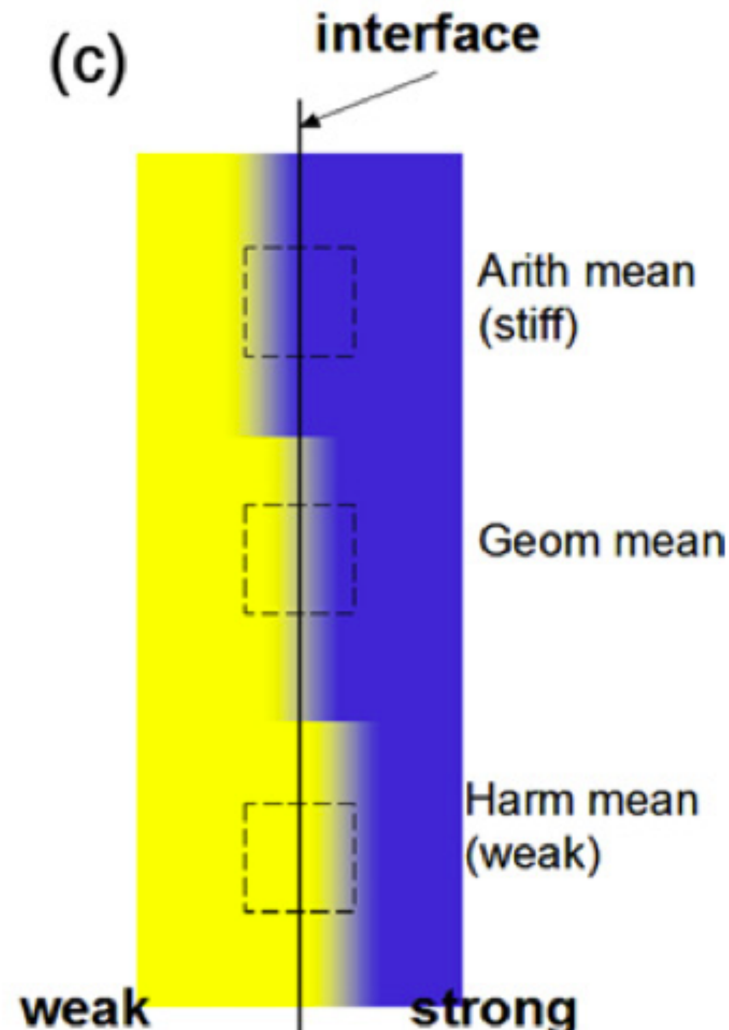
- Averaging affects rheological boundaries

Schmeling et al. (2008):
- Harmonic → equivalent to effective viscosity of 2 viscous elements acting in series, like channel flow with flow-parallel compositional boundary, i.e. simple shear. Results in weak effective viscosity.
- Arithmetic → 2 viscous elements in parallel, interface-parallel pure shear. Results in stiff effective viscosity.
- Geometric norm has no physical model, intermediate viscosity.

→ Harmonic mean more appropriate for high viscosity contrasts (1e4) and flows dominated by cusp-like overriding wedges

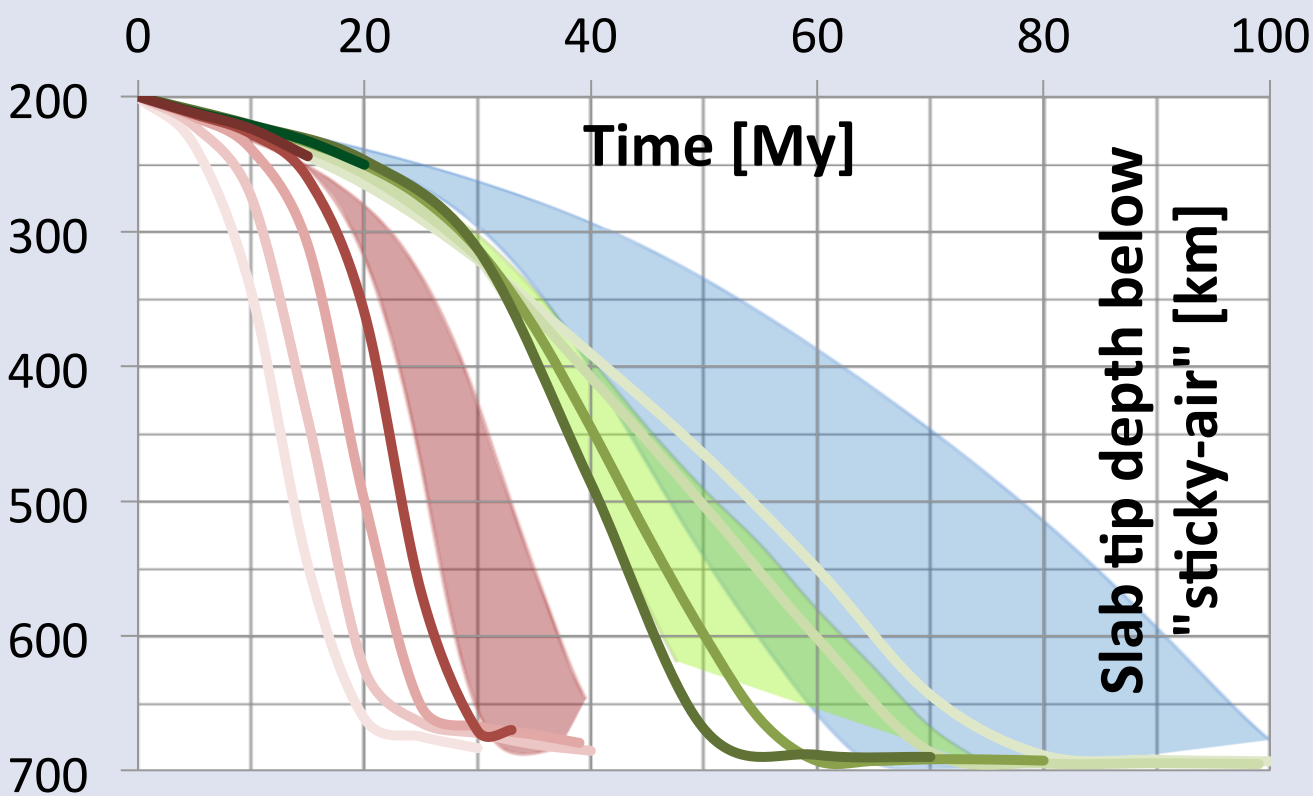


Schmeling et al., PEPI, 2008

Subduction evolution

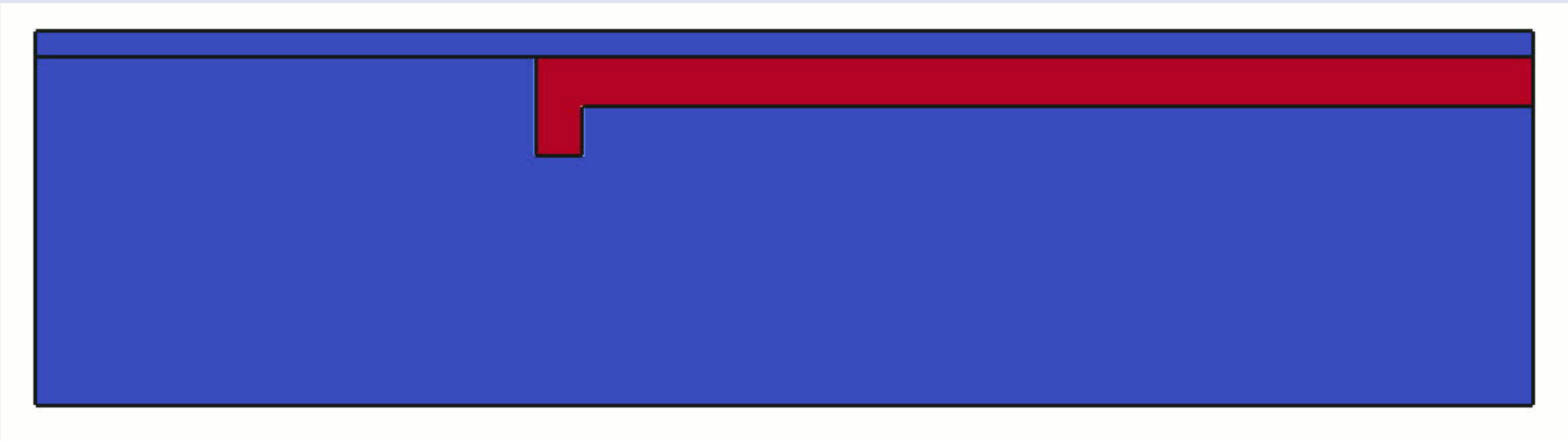
Harmonic: higher resolution, slower subduction

Geometric: higher resolution, faster subduction



Shaded areas from Schmeling et al., PEPI, 2008, lines obtained with ASPECT

Results harmonic averaging

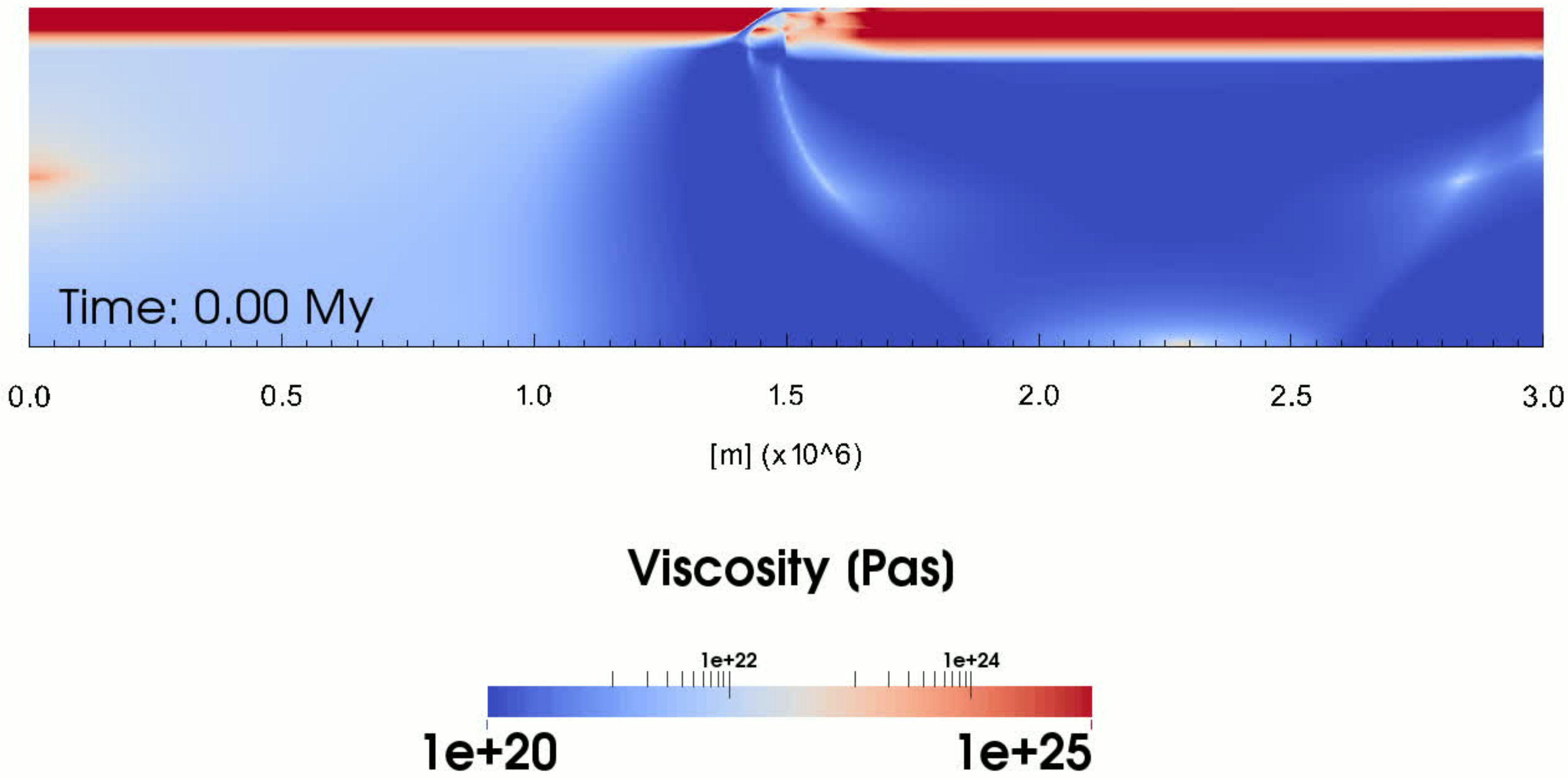


Red colors indicate composition 2

Extending on subduction models

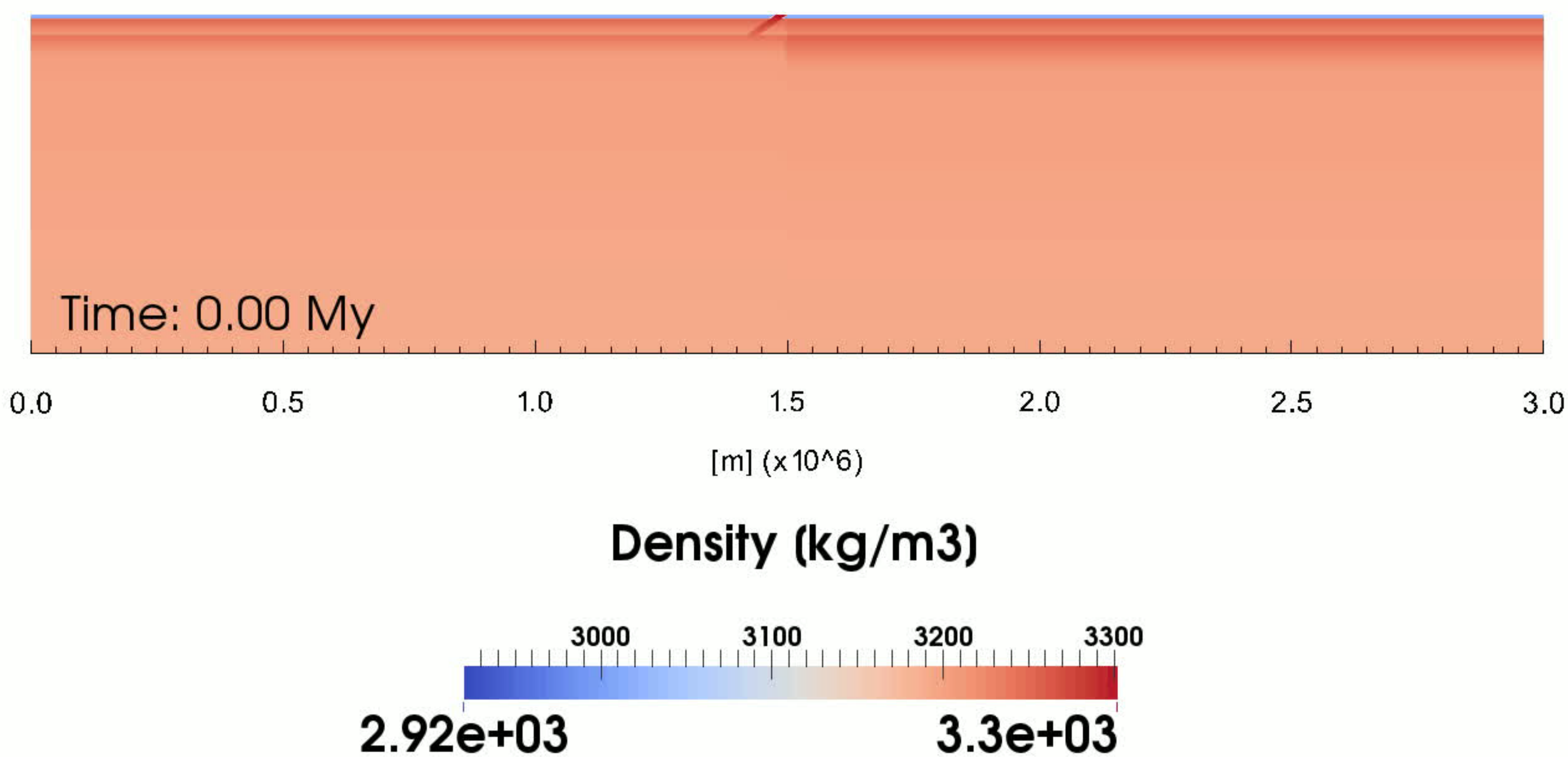
- More materials with different characteristics, i.e. overriding plate and crust
- Realistic deformation mechanisms, i.e. elasto-visco-plasticity
- Complex boundary conditions, i.e. plate velocities, free surfaces, open boundaries
- 4D modeling

Example – Quinquis et al. (in prep)



ASPECT 2014 – visco-plastic, thermo-mechanically coupled subduction, 8 materials

Example – Quinquis et al. (in prep)



ASPECT 2014 – visco-plastic, thermo-mechanically coupled subduction, 8 materials