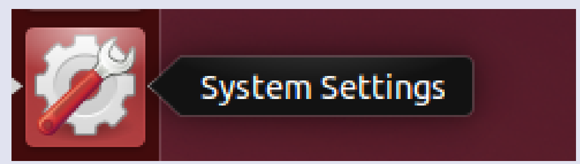
Before you start the virtual machine:

- In Virtual Box: “Settings” → “System” → “Processor” tab → pick number of CPUs (2 or 4)
- Start your virtual machine and log into the aspect_user account
- Click on the gear symbol (“System Settings”)



- Click on “Brightness & Lock”
- Set: “Turn screen off when inactive for:” to “Never”
- Turn “Lock” slider to “off”

ASPECT tutorial

Wolfgang Bangerth
Juliane Dannberg
Rene Gassmöller
Timo Heister

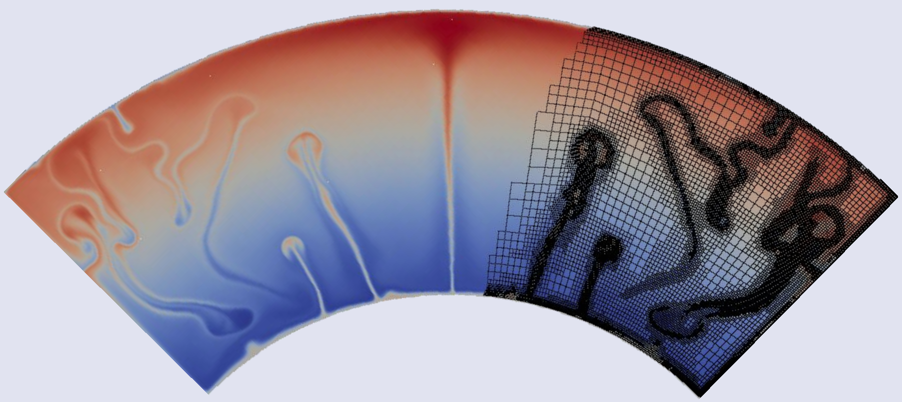
Lecture 0
First Steps
Running ASPECT

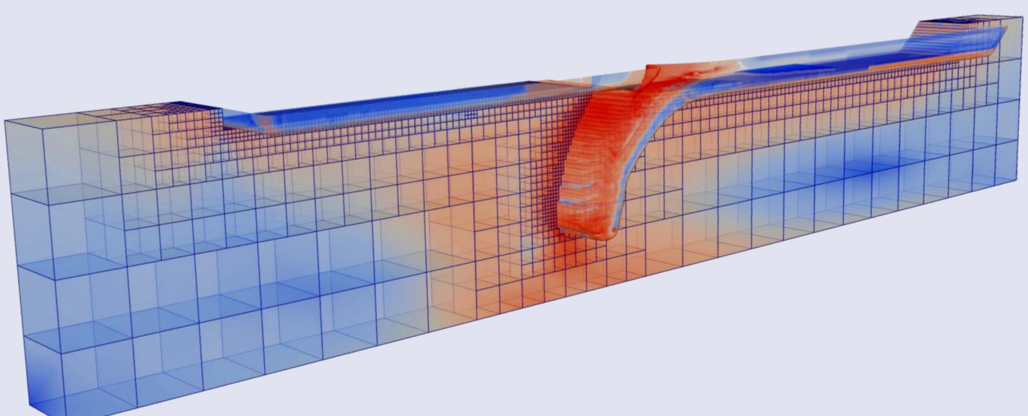
What is Aspect?

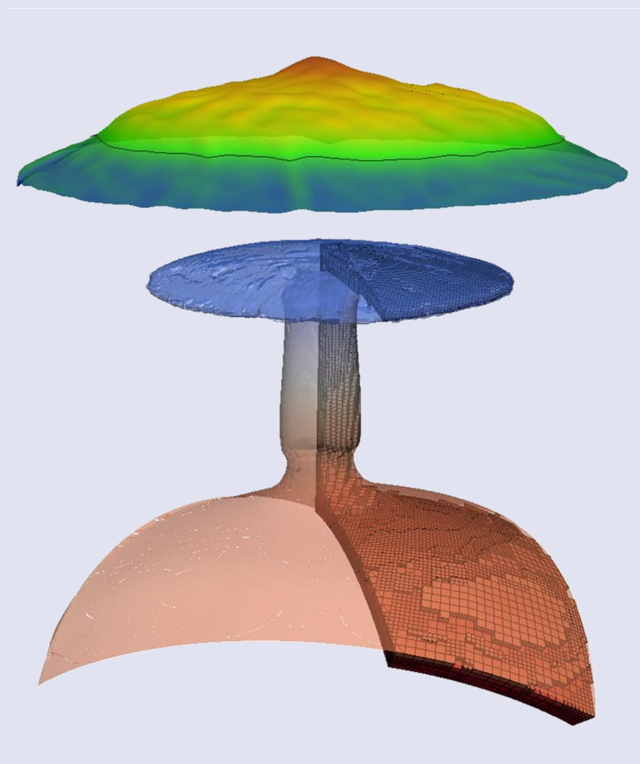
CIG COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

ASPECT

- Advanced Solver for Problems in Earth's ConvecTion -







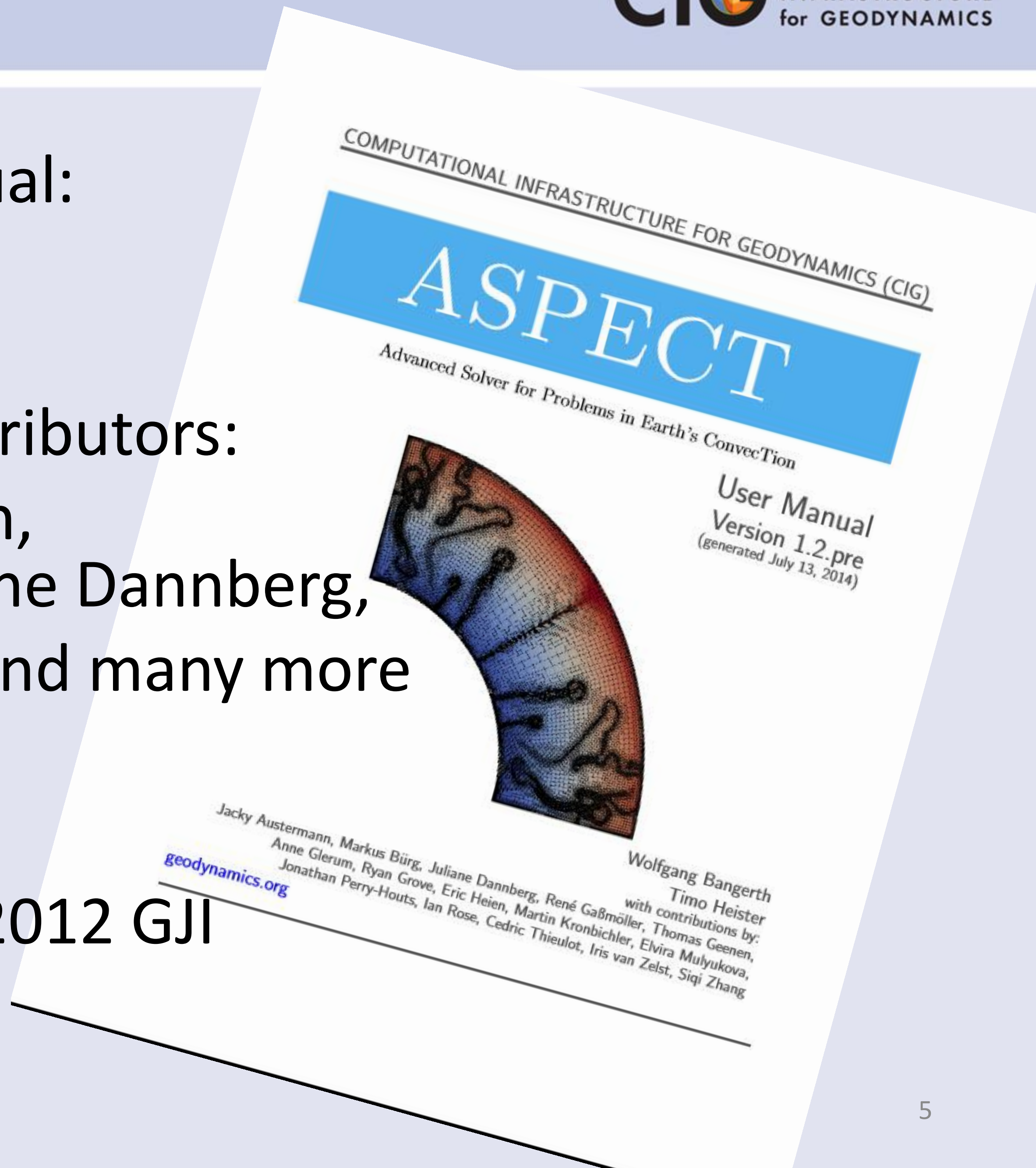
Credits

CIG COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

Website and manual:
aspect.dealii.org

Developers & contributors:
Wolfgang Bangerth,
Timo Heister, Juliane Dannberg,
Rene Gassmöller and many more

Publication:
Kronbichler et al. 2012 GJI



Using ASPECT

- Basic usage of ASPECT is specified through a parameter file
- 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 should 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.

Using ASPECT

- We will begin by running ASPECT in the Terminal

1. Change to the appropriate directory

```
cd Desktop
```

2. Run ASPECT with the tutorial parameter file and print the output to a file named progress.txt (this will take about 20 seconds)

```
./aspect tutorial.prm | tee progress.txt
```

3. Open progress.txt and check the Rayleigh number

```
gedit progress.txt
```

Debug or Optimized mode?

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

- When you start ASPECT…

```
-----------------------------------------------------------------------------
-- This is ASPECT, the Advanced Solver for Problems in Earth's ConvecTion.
--      . version 1.2.pre
--      . running in OPTIMIZED mode
--      . running with 1 MPI process
--      . using Trilinos
-----------------------------------------------------------------------------
```

DEBUG or OPTIMIZED

TRILINOS or PETSc

```
ccmake .
```

```
                                             Page 1 of 1
 ASPECT_USE_PETSC                OFF
 CMAKE_BUILD_TYPE                Release
 deal.II_DIR                     /home/aspect/ASPECT_TUTORIAL/deal.II-8.1/lib/cmake/deal.II




ASPECT_USE_PETSC: Use PETSc instead of Trilinos if set to 'on'.
Press [enter] to edit option
Press [c] to configure
Press [h] for help           Press [q] to quit without generating
Press [t] to toggle advanced mode (Currently Off)
```

Visualizing Results with ParaView

Visualization with ParaView

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

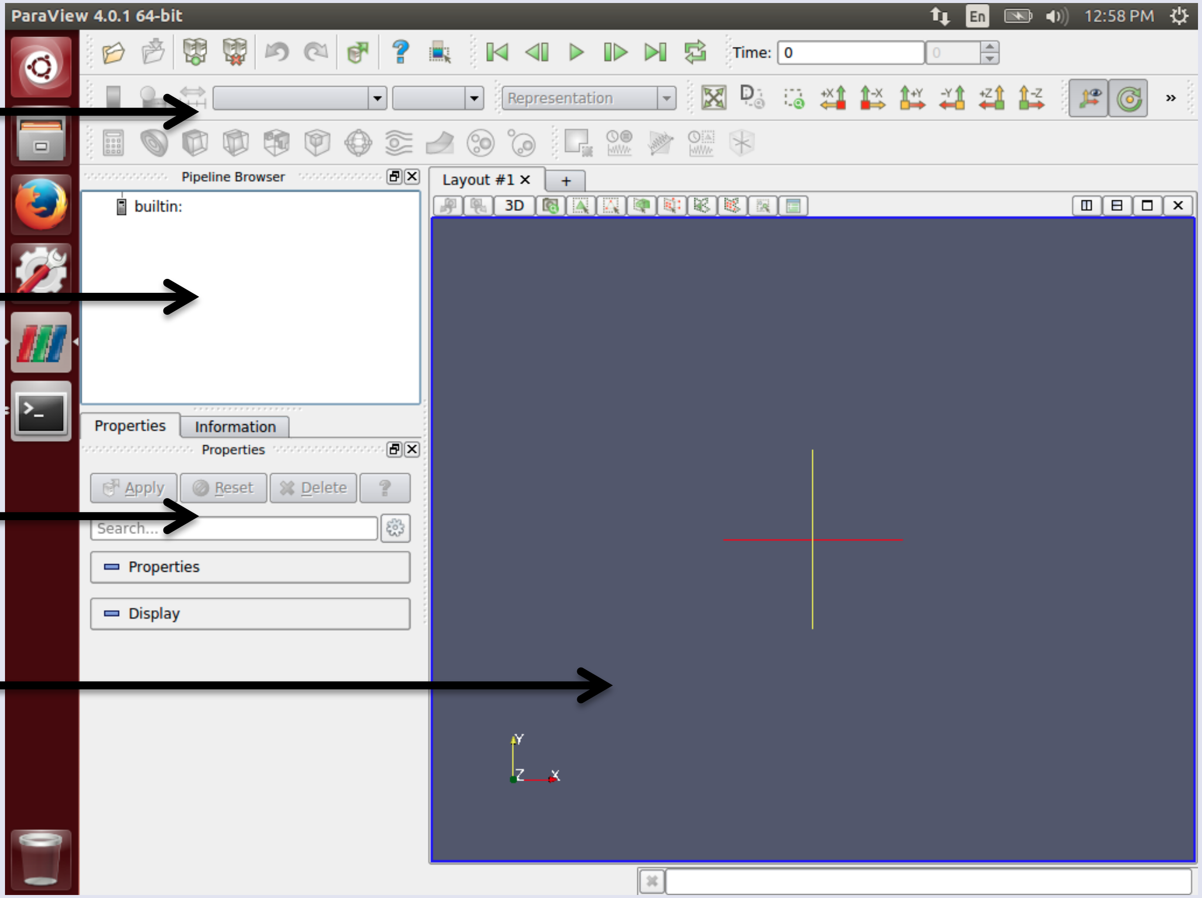
Visualization with ParaView

Toolbars

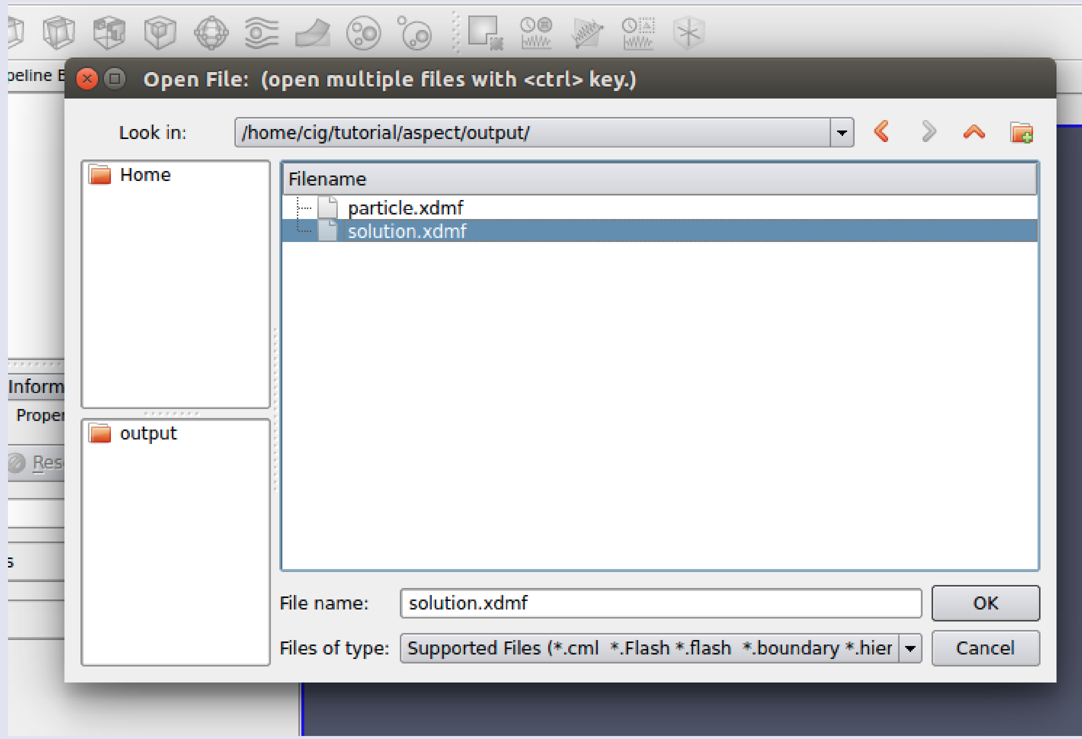
Pipeline Browser

Object Inspector

2D/3D View



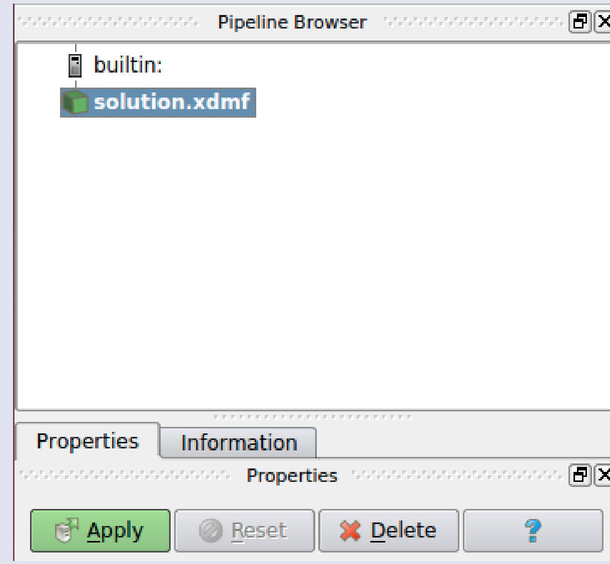
Visualization with ParaView

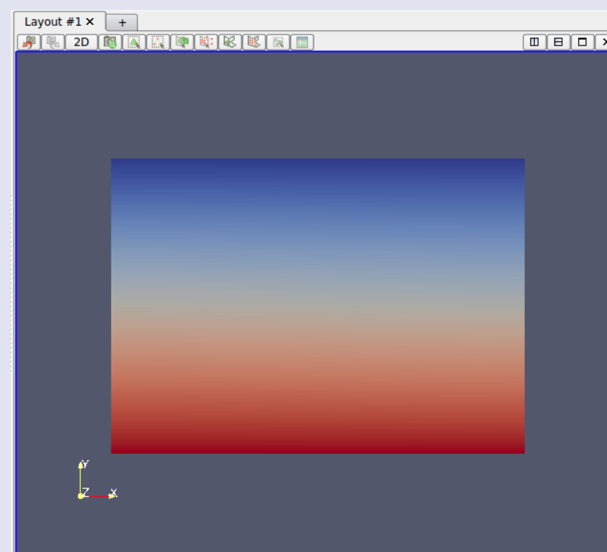


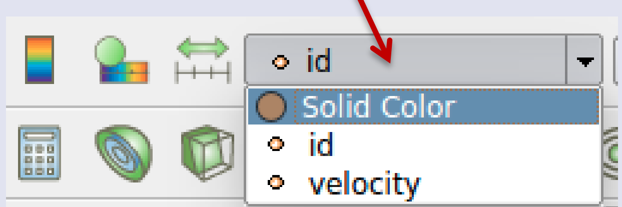
- Start by opening solution.pvtu which was created by running ASPECT
- You can choose “Open” from the File menu or use the Open icon  in the toolbar
- The file is in /home/aspect_user/Desktop/output/

Visualization with ParaView

- The file will appear in the pipeline browser
  - Make sure this is solution.pvd
- The list of properties (variables) appears in the object inspector
  - The file contains temperature (T), pressure (p), and velocity
- Click “Apply” to show the field in the view area
  - By default, no field is shown
  - Select “T” in the toolbar to show the temperature field







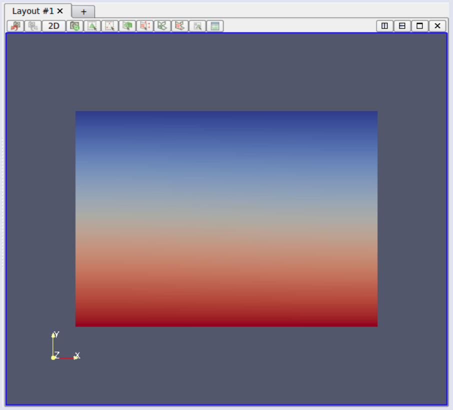
Visualization with ParaView

CIG COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

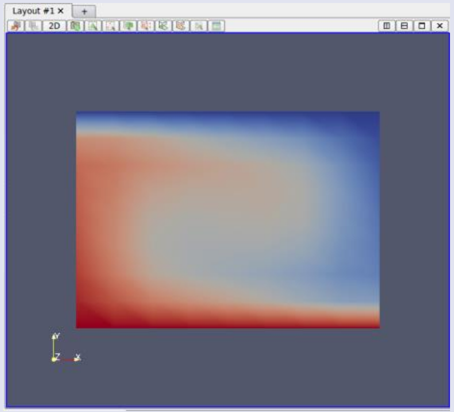
- The top toolbar has buttons to change the time, shown below
  - Click the play button and watch how the temperature field changes
  - Near the end, is the temperature field static? Is the velocity field static? Is material moving?

Previous Frame | Next Frame | Loop

First Frame | Play/Pause | Last Frame | Simulation Time | Time step number



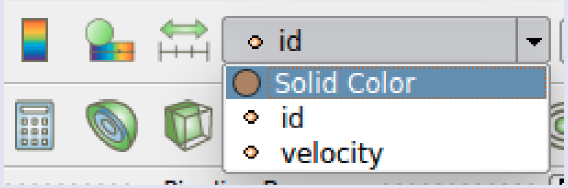
Frame 0



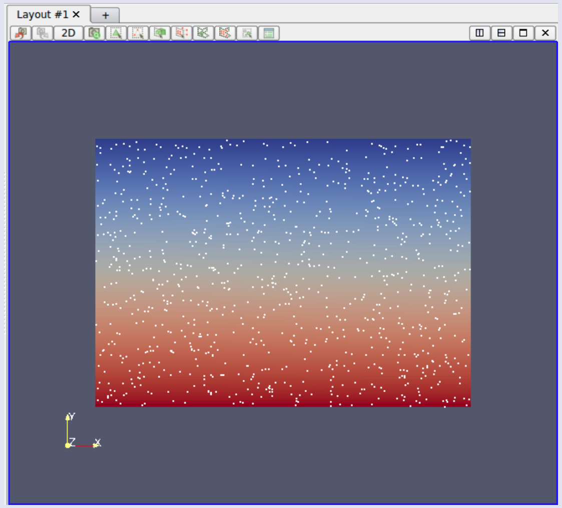
Frame 231

Visualization with ParaView

- Open the file particle.pvd and click "Apply"
  - The tracer particles from the simulation now appear on the temperature field
  - By default they are uniformly colored
  - Click play again to see how material is flowing with the tracer particles
  - Even when the temperature field is static, is material flowing?
  - How would you characterize this flow pattern? Where is the upwelling material? The downwelling material?



Change the coloring scheme to "Solid Color"



Temperature field with tracer particles

Lecture I
ASPECT – A Next-generation geodynamic modeling software

Juliane Dannberg

Equations and models, and how they are represented in ASPECT

Setup of the numerical model

- Numerical models generally consist of several key components:
  1. The rules (e.g. equations) for the model
  2. The discretization of the model
  3. Model parameters
  4. Dependent and independent variables
  5. The initial state of the model
  6. The boundary conditions
- We will go through the parameter file and look at these components

```
gedit tutorial.prm
```

ASPECT - General

- First we look at general parameters for the simulation
- Dimension=2 specifies a two dimensional problem
- Internally, the calculations will use seconds, but the output will be represented in years
  - This helps to understand processes on Earth time scales
- End time has been set to 5×10^{10} years.
  - Side note: computers often use E notation, such that 2×10^{3} is written 2E3
  - Hence we write 5e10 or 5E10 rather than 5×10^{10}
- Simulation output will be stored in the directory named "output".

```
3     set Dimension                                  = 2
8     set Use years in output instead of seconds     = true
9     set End time                                   = 5e10
10    set Output directory                           = output
```

Equations

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

Momentum equation

Divergence of stress tensor

Only viscous stress (no elasticity/plasticity), no inertia

Pressure gradient

Gravity force

(Total pressure instead of only dynamic pressure)

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

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	$\frac{W}{kg}$

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

Includes compressibility

$\mathbf{u}$	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	$\frac{W}{kg}$

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

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

$$-\frac{\partial \rho}{\partial T} T \mathbf{u} \cdot \mathbf{g}$$

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

Change of energy over time

Advection

Heat conduction

Radiogenic heating

Shear heating

Adiabatic heating $\frac{\partial \rho}{\partial T} = -\rho \alpha$

latent heat (phase changes)

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

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

$$-\frac{\partial \rho}{\partial T} T \mathbf{u} \cdot \mathbf{g} \quad + \rho T \cdot \Delta S \frac{DX}{Dt}$$

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

Advection of compositional fields

Field method (or tracer method)

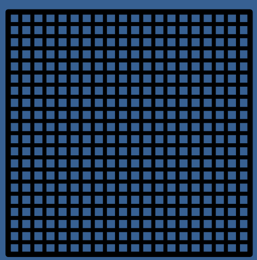
Summary of equations

- Compressibility
- 2- or 3-dimensional domain Ω, different geometries
- Total pressure
- Radiogenic heating
- Adiabatic heating, shear heating & latent heat
- Advection of any number of compositional fields

Geometry model

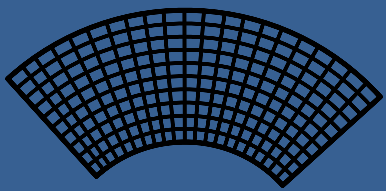
2D or 3D?

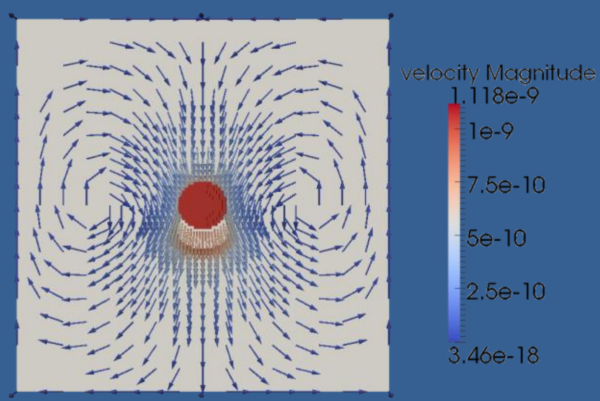
Geometry model

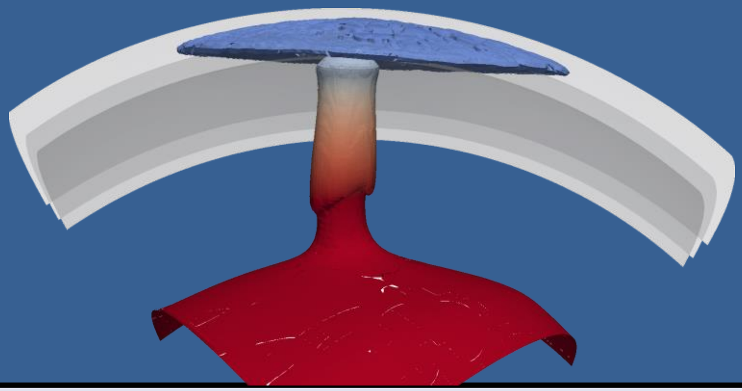


Box

Spherical shell



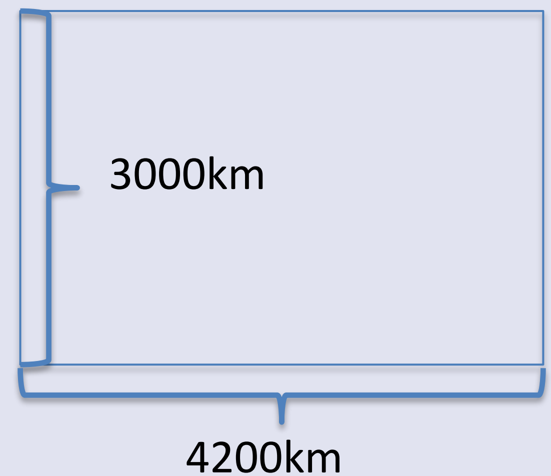




ASPECT - Geometry

- Aspect has many built in geometry models such as “box” and “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.

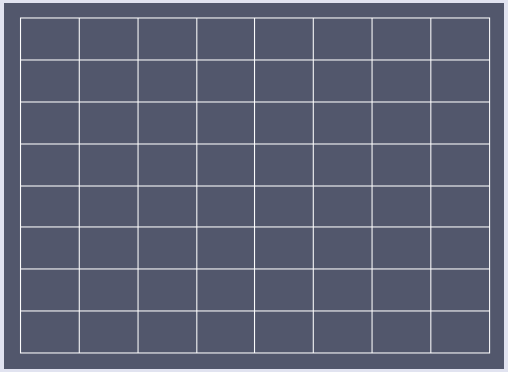
Simulation Model



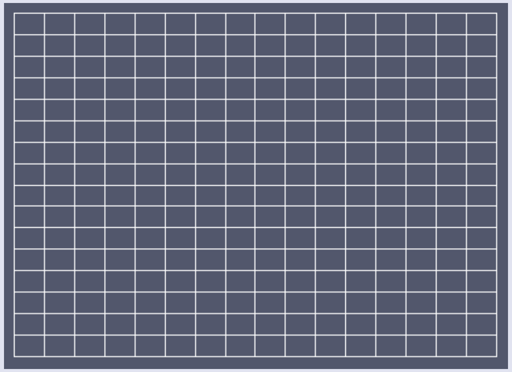

```
subsection Geometry model
        set Model name = box
        subsection Box
                set X extent = 4.2e6
                set Y extent = 3e6
        end
end
```

ASPECT - Discretization

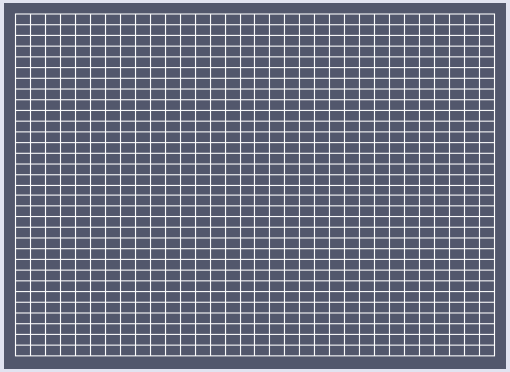
- Initial global refinement specifies the “grid spacing” of our mesh.
- For this tutorial, REFINE=3 or 4 or 5.
- Adaptive mesh refinement has been turned off, i.e. the mesh does not change during the simulation.



REFINE=3 (8x8 cells)



REFINE=4 (16x16 cells)

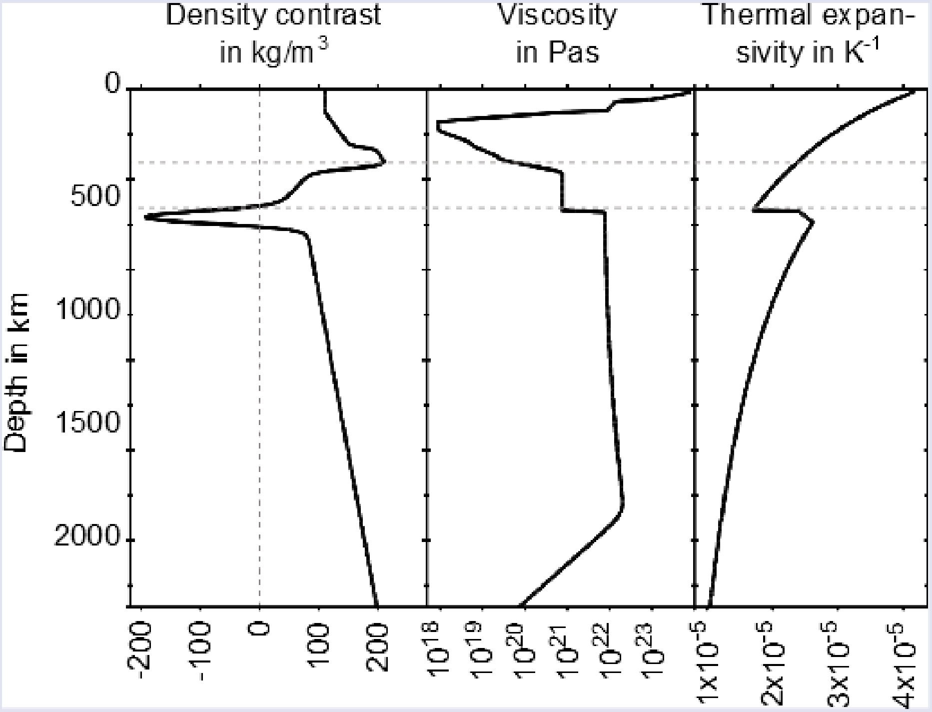


REFINE=5 (32x32 cells)

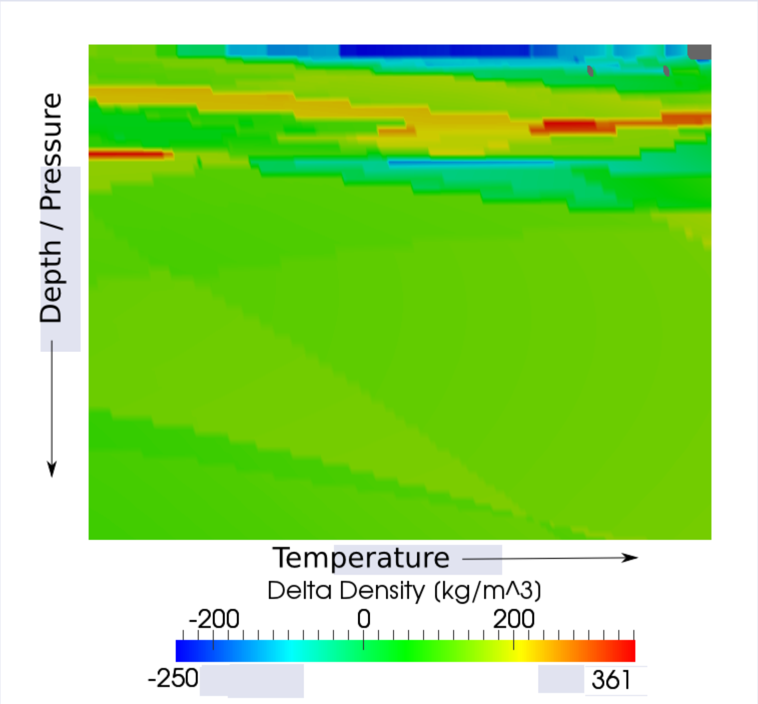
```
subsection Mesh refinement
    set Initial global refinement = REFINE
    set Initial adaptive refinement = 0
    set Time steps between mesh refinement = 0
end
```

Material model

Input:
Temperature, pressure, composition, strain rate, position



Parameterization



Lookup table from Perplex / HeFESTo

ASPECT - Model Parameters

CIG COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

- Aspect provides various built in material models, and a framework for users to implement custom material models.
- In this tutorial, you control the Rayleigh number with the viscosity parameter.
- There are several other parameters which control reference density, temperature dependence of viscosity, etc. These have default values shown below.

$$Ra = \frac{\rho_0 g \alpha \Delta T D^3}{\eta \kappa}$$

$$\eta = \frac{\rho_0 g \alpha \Delta T D^3}{\kappa Ra} = \frac{5.0993 \times 10^{28}}{Ra}$$

Default Values

$$\rho_0 = 3300, g = 9.8, \alpha = 2 \times 10^{-5}, \Delta T = (3600 - 273) = 3327$$

$$D = 3 \times 10^6, k = 4.7, c_p = 1250, \kappa = \frac{k}{\rho_0 c_p} = 1.1394 \times 10^{-6}$$

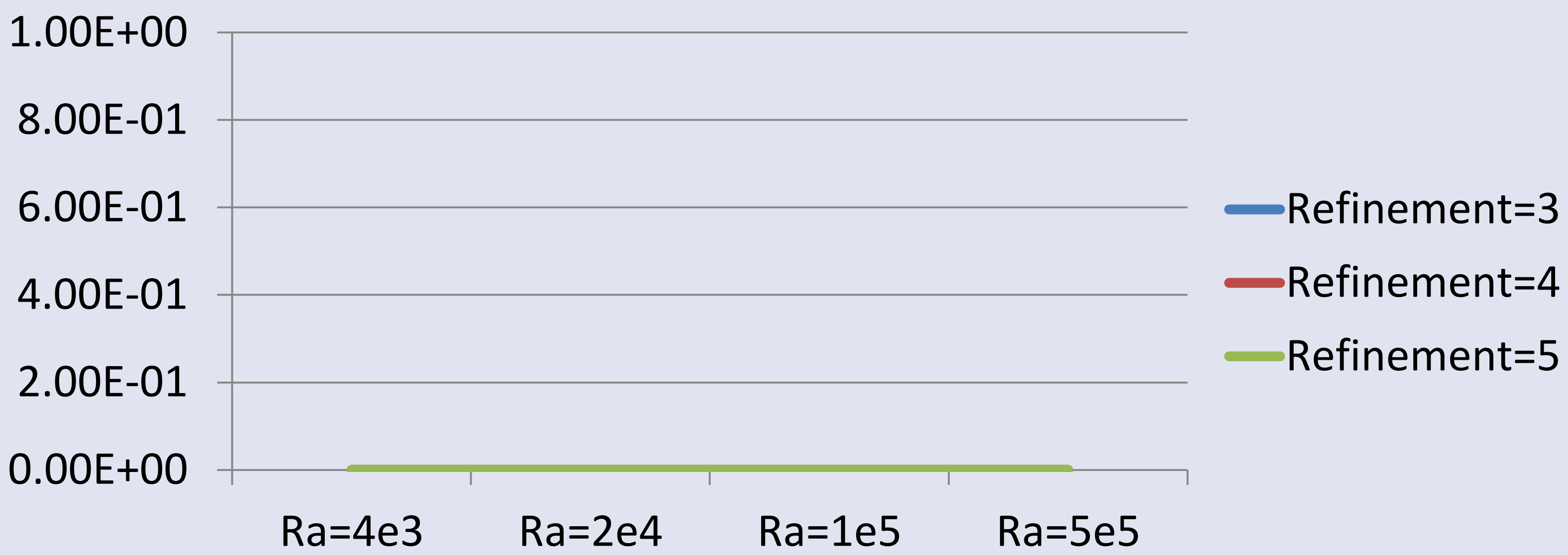
```
subsection Gravity model
   set Model name = vertical
   subsection Vertical
     set Magnitude = 9.8
   end
 end
```

```
subsection Material model
         set Model name = simple
         subsection Simple model
             set Viscosity = VISCOSITY
         end
end
```

Nusselt-Rayleigh Relationship

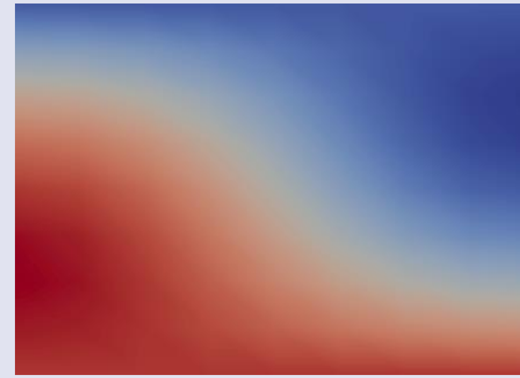
COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

	Ra=4,000	Ra=20,000	Ra=100,000	Ra=500,000
End Time	1e12	2e11	3e10	5e9
Viscosity	1.275E25	2.550E24	5.099E23	1.020E23
Refine = 3	(???)	(???)	(???)	(???)
Refine = 4	(???)	(???)	(???)	(???)



ASPECT - Initial Conditions

- Aspect has initial condition models to specify the temperature initial conditions and framework for users to implement custom initial condition models.
- The function model lets us specify the initial temperature as a mathematical formula, with user defined constants.
- Here we are specifying a sinusoidal perturbation of a linear temperature profile.

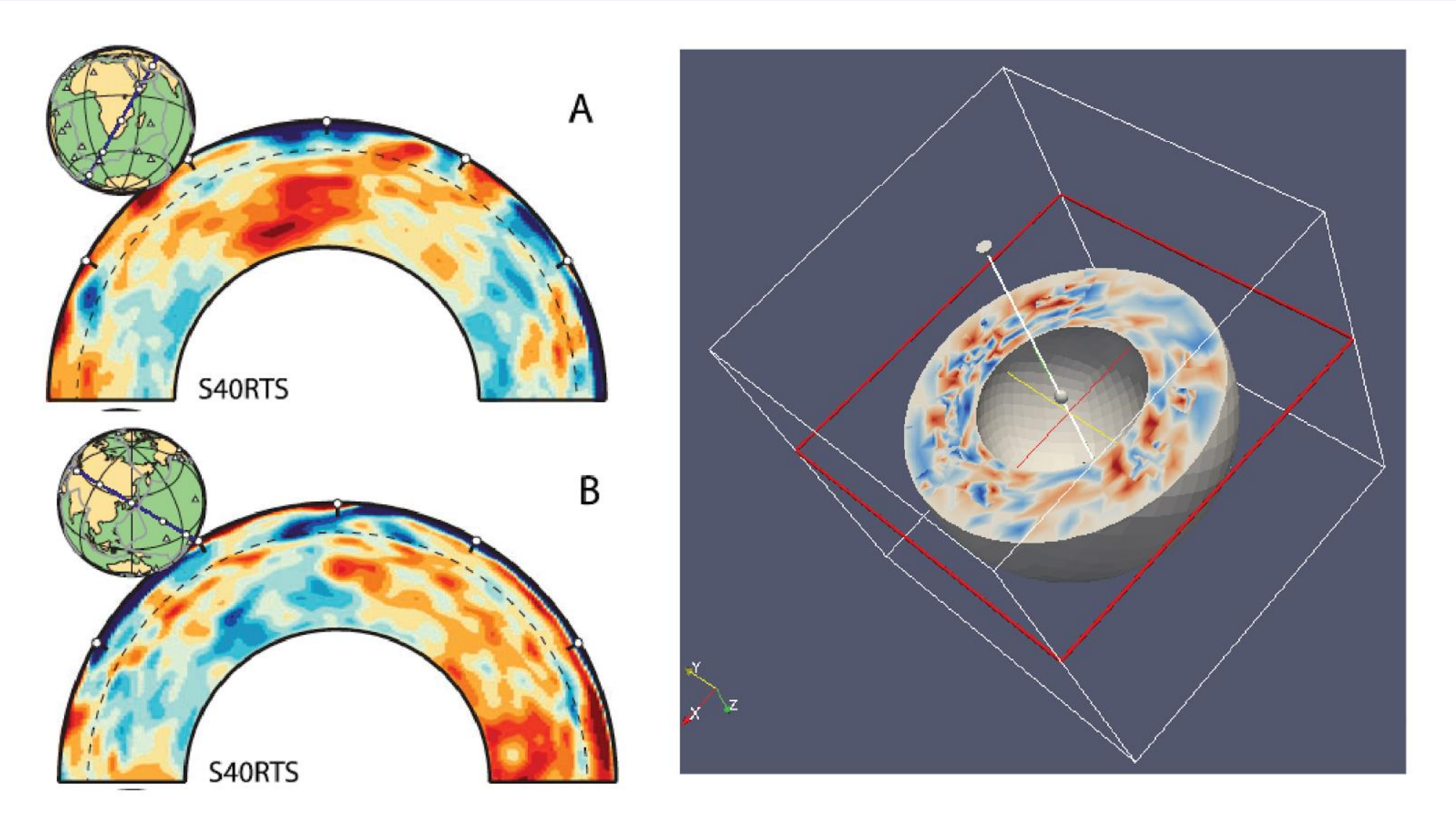


Initial temperature field (p=-0.5)

$$T(x,y) = T_{top} + (T_{bottom} - T_{top})(1 - \frac{y}{D} - pcos(\frac{k\pi x}{L})sin(\frac{\pi y}{D})$$

```
subsection Initial conditions
        set Model name = function
        subsection Function
                set Variable names = x,y
                set Function constants = p=-0.01, L=4.2e6, D=3e6,
                        pi=3.1415926536, k=1, T_top=273, T_bottom=3600
                set Function expression = T_top + (T_bottom-T_top)*
                        (1-(y/D)-p*cos(k*pi*x/L)*sin(pi*y/D)))
        end
end
```

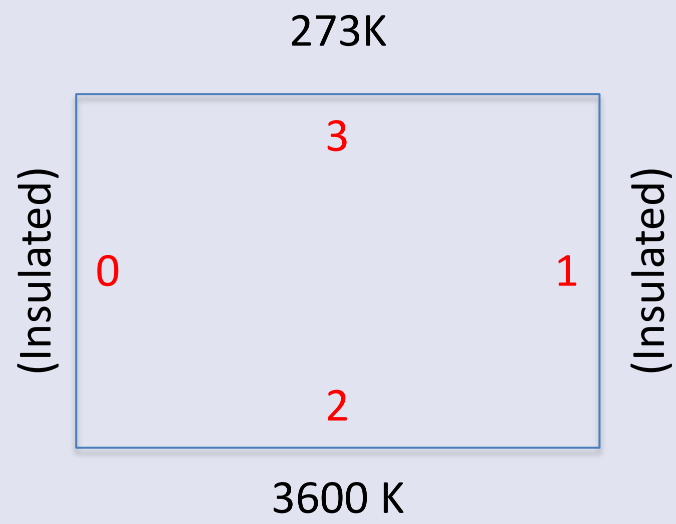
Seismic models as initial condition



From J. Austermann

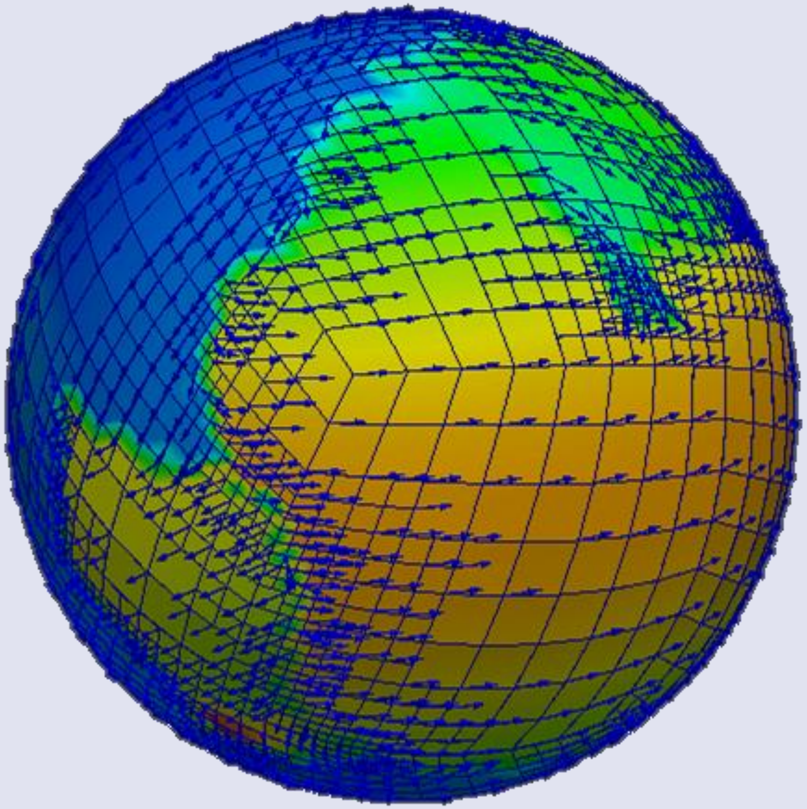
ASPECT - Boundary Conditions

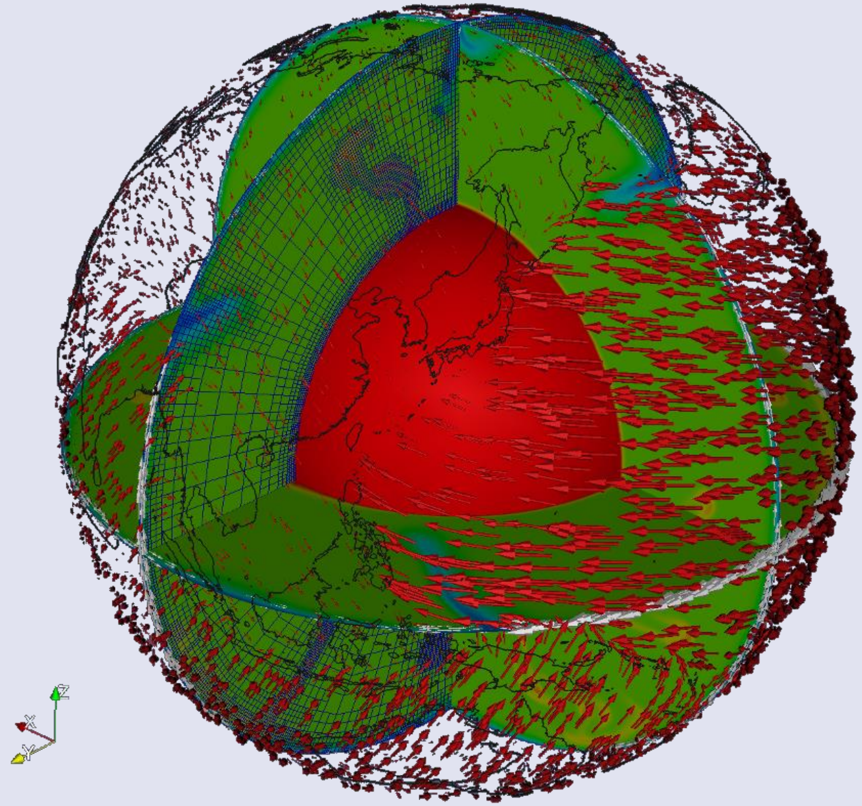
- The temperature at the bottom of the box is fixed at 3600 K, top is 273K
- Depending on the model, Left and Right options can be similarly specified (and front/back in 3D)
- If unspecified, the boundaries default to no heat flux (insulated)
- All boundaries (0,1,2,3) are free-slip
- Geometry models also provide symbolic names for each boundary part




```
subsection Model settings
   set Fixed temperature boundary indicators   = 2,3
   set Zero velocity boundary indicators       =
   set Prescribed velocity boundary indicators =
   set Tangential velocity boundary indicators = 0,1,2,3
end
subsection Boundary temperature model
set Model name = box
           subsection Box
                      set Bottom temperature = 3600
                      set Top temperature = 273
           end
end
```

Boundary conditions model





From R. Gassmoeller

GPlates

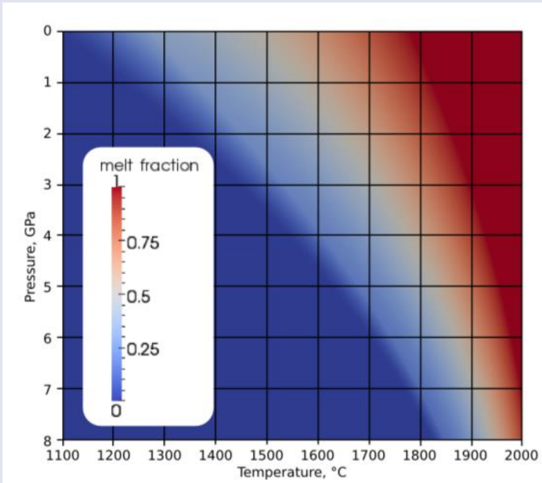
ASPECT - Postprocessing

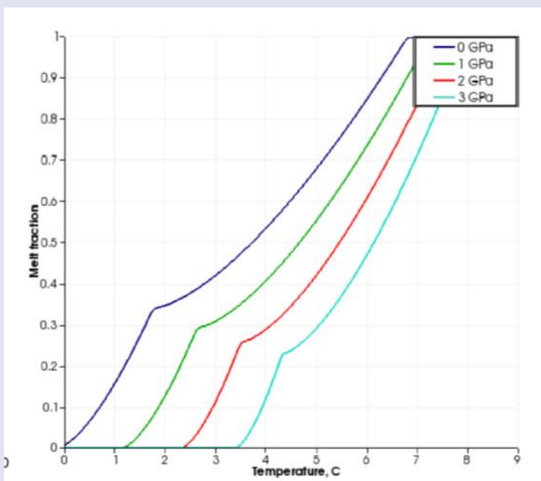
- This section of the parameter file specifies how to analyze the data that has been generated.
- Heat flux statistics and visualization will be used in this tutorial.
- Graphical output is generated every 1e7 simulated years
- We will also add tracer particles to better understand the flow pattern

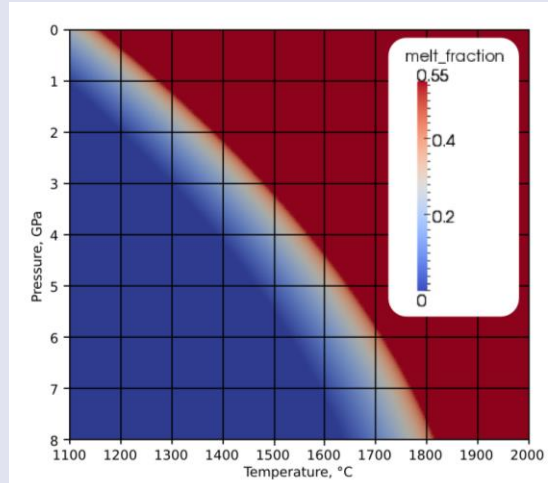
```
subsection Postprocess
    set List of postprocessors = velocity statistics, temperature
                                 statistics, heat flux statistics
    subsection Visualization
        set Time between graphical output = 1e7
        set Output format = hdf5
    end
    subsection Tracers
        set Number of tracers = 1000
        set Time between data output = 1e7
        set Data output format = hdf5
  end
end
```

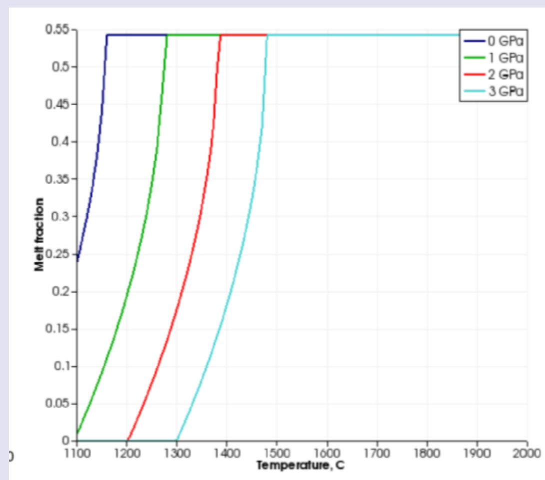
Melt fraction postprocessor

Peridotite
(after Katz et al., 2003)



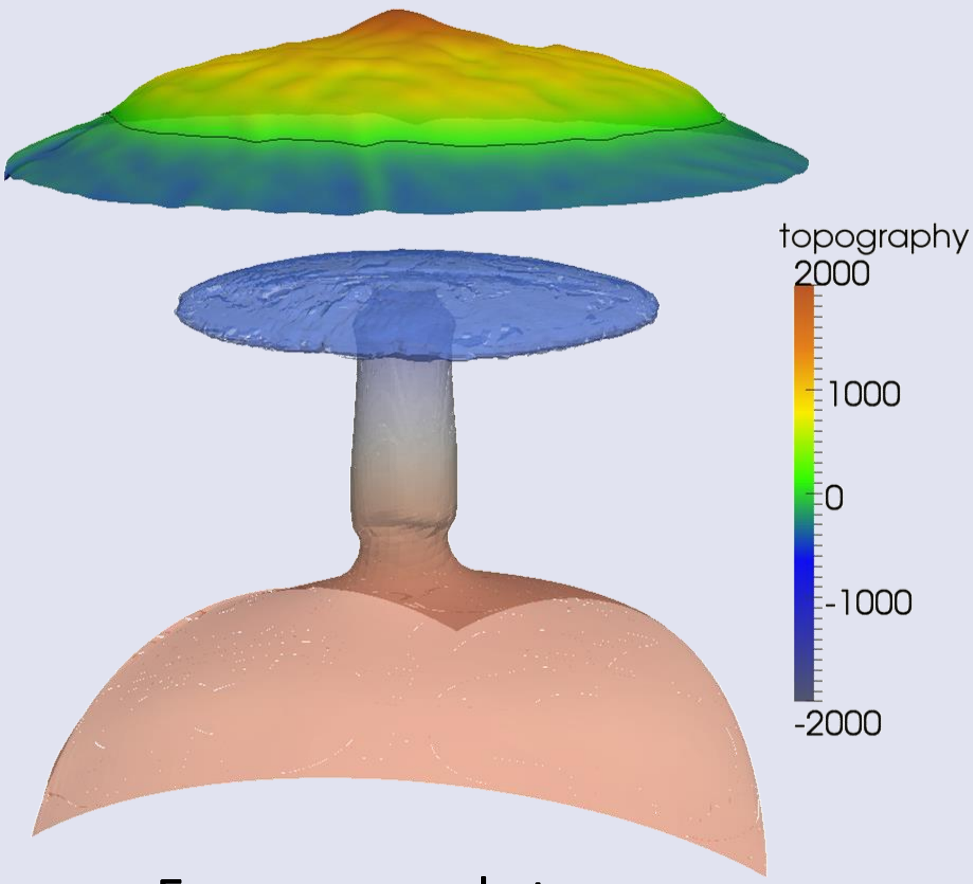






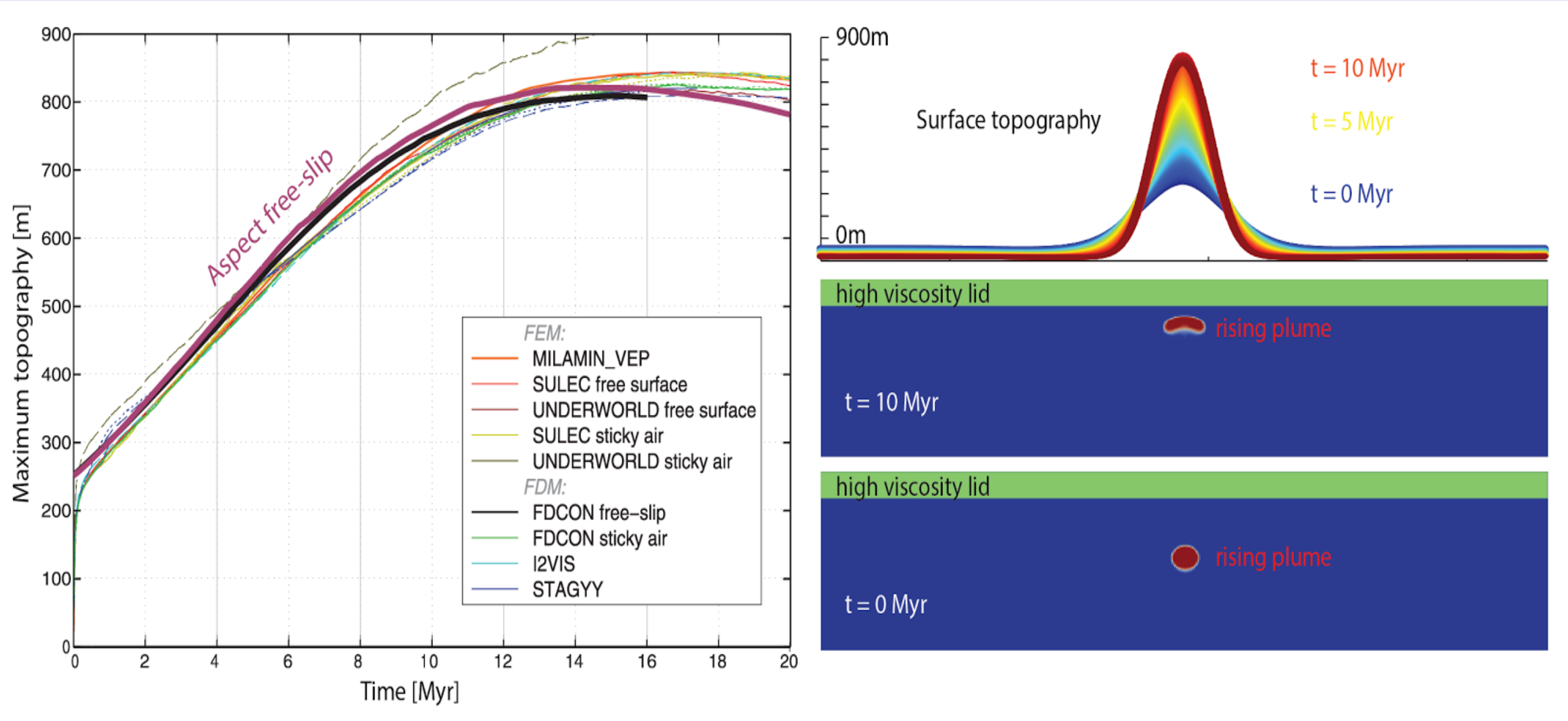
Pyroxenite
(after Sobolev et al., 2011)

Surface topography



From normal stress

Topography: free-slip (Crameri et al, 2012)



Work with J. Austermann

Topography: Free Surface

- Using an arbitrary Lagrangian-Eulerian framework

Equations for moving the mesh nodes:

$$\begin{aligned} -\Delta \mathbf{u}_m &= 0 && \text{in } \Omega \\ \mathbf{u}_m &= (\mathbf{u}\cdot\mathbf{n})\,\mathbf{n} && \text{on } \partial\Omega_{\text{free surface}} \\ \mathbf{u}_m \cdot \mathbf{n} &= 0 && \text{on } \partial\Omega_{\text{free slip}} \\ \mathbf{u}_m &= 0 && \text{on } \partial\Omega_{\text{Dirichlet}} \end{aligned}$$

Modification of the advection equation:

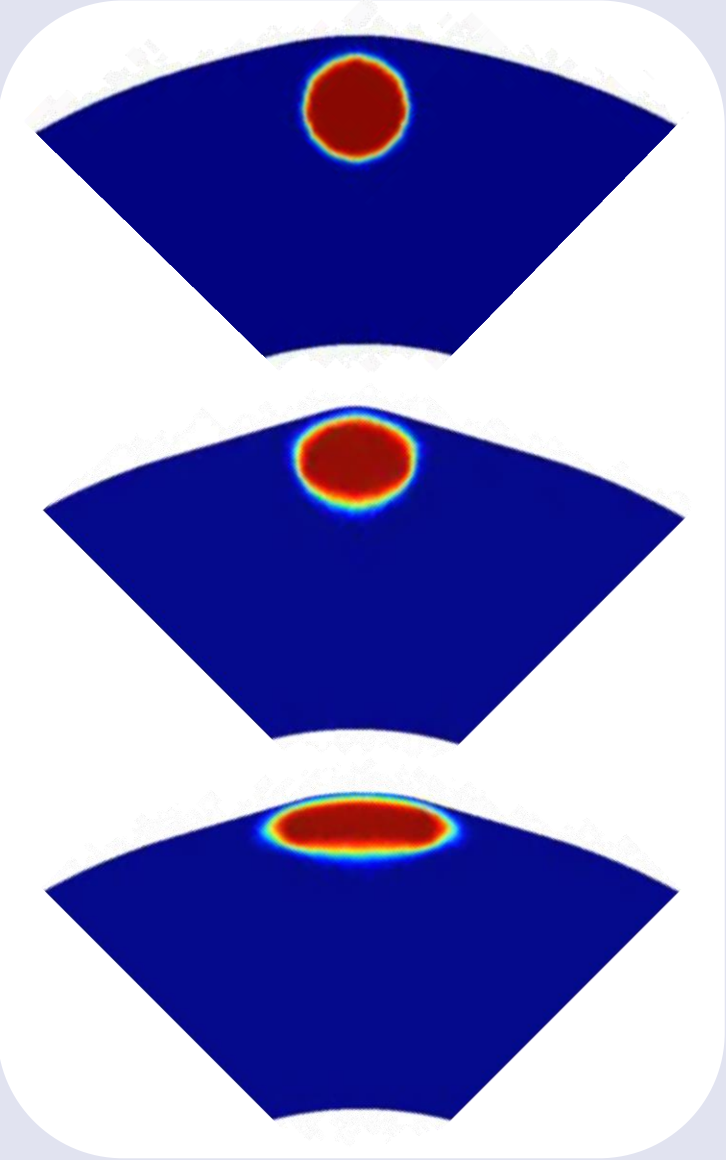
$$\rho C_p \left(\frac{\partial T}{\partial t} + (\mathbf{u} - \mathbf{u}_m)\cdot \nabla T \right) - \nabla \cdot k \nabla T = \rho H \quad \text{in } \Omega$$

Using the stabilization of:

Boris JP Kaus, Hans Mühlhaus, and Dave A May. A stabilization algorithm for geodynamic numerical simulations with a free surface. *Physics of the Earth and Planetary Interiors*, 181(1):12–20, 2010.

From I. Rose

Free surface



From I. Rose

ASPECT as software:
Philosophy and numerical methods

Codes in Geodynamics

- There are some widely used codes
- Almost all codes use globally refined meshes
- Almost all codes use lowest order elements
- Most codes use “simple” solvers
- No code has been “designed” with a view to
  – extensibility
  – maintainability
  – correctness

Geodynamics: Design challenges

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

As a "community code", *Aspect* needs to satisfy these goals:

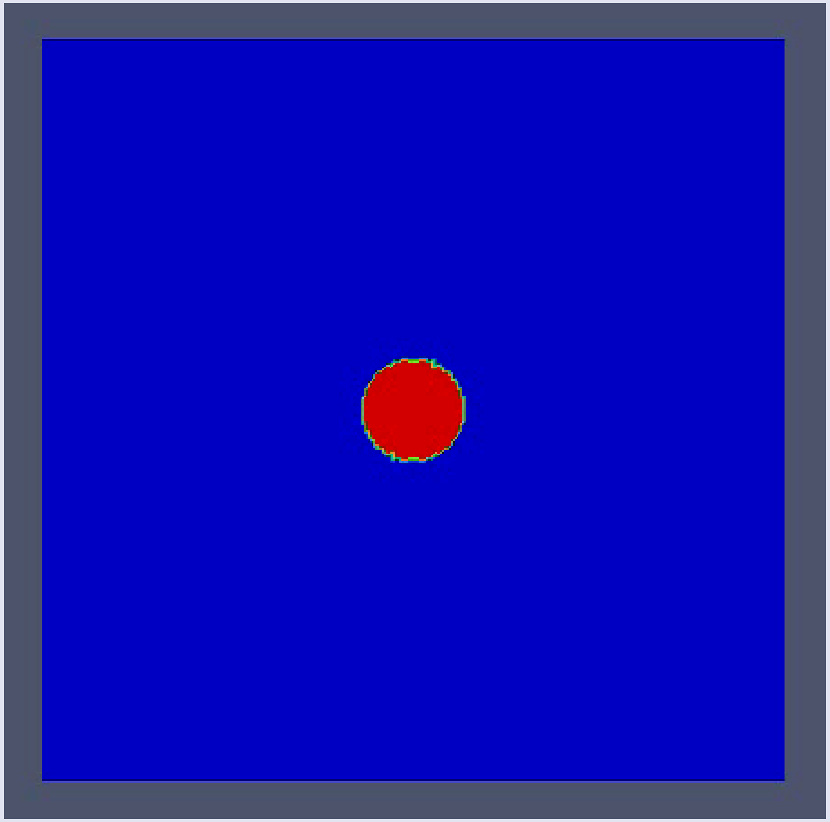
- Can solve problems of interest (to geodynamicists)
- Be well tested
- Use modern numerical methods
- Be very easy to extend to allow for experiments
- Freely available

Numerical methods

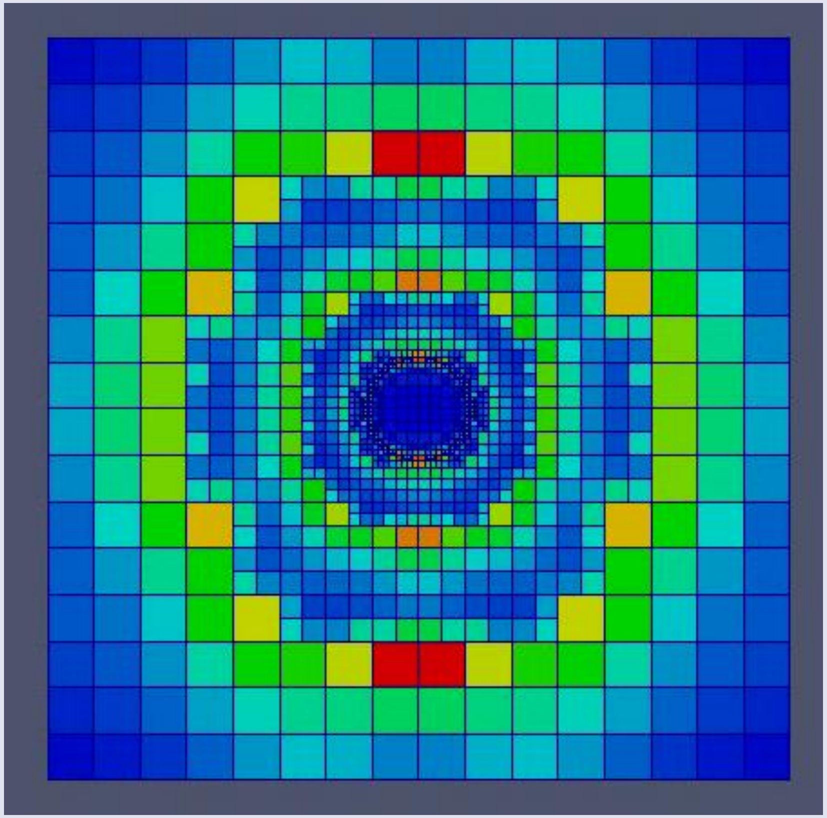
- Mesh adaptation
- Accurate discretizations (choice of finite element for velocity and pressure + nonlinear artificial diffusion for temperature stabilization)
- Efficient linear solvers (preconditioner + algebraic multigrid)
- Parallelization of all of the steps above
- Modularity of the code

Mesh adaptation

- Example: Composition as refinement strategy



Compositional field



Mesh cells, colors indicate the estimated error

Mesh adaptation

Choose **Strategies**:
temperature, density, velocity, composition, thermal energy density

Calculate error estimate c_K (based on 2nd derivatives & cell diameter)

$$E = \sum_{K \in T} c_K$$

Total error estimate E

Normalize refinement criteria?

Scale errors for each criterium?

Add errors/take maximum?

Choose **refinement + coarsening fraction** *a*

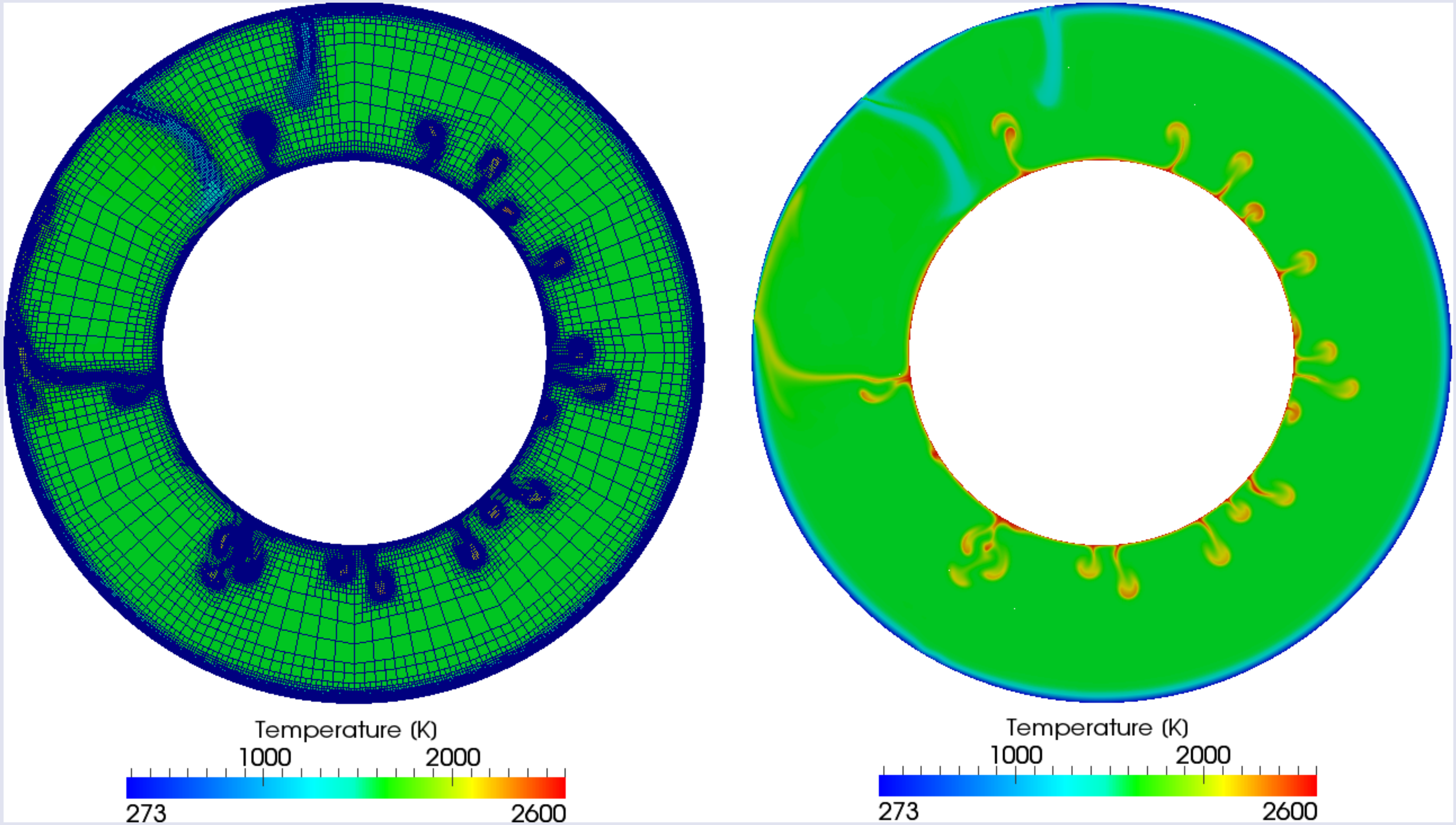
Look for the smallest subset M

$$aE = \sum_{K \in M} c_K$$

(sum up c_K in the cells with the largest/smallest error until you reach fraction *a* of the error)

Mark those cells for refinement/coarsening

Mesh adaptation



Discretization

- Finite element method
- Uses Cartesian coordinates (mapping for curved boundaries)
- Free choice of finite element basis functions
- Stability: choose polynomial degree of velocity one order higher than for pressure (e.g. linear and quadratic)

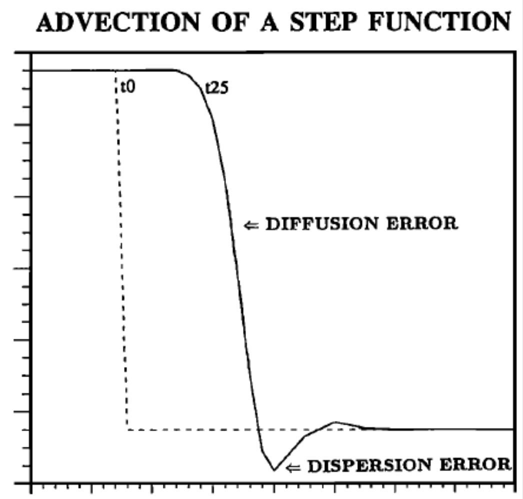
Pressure

Velocity, temperature, composition

Discretization of temperature

- Problem: high gradients and low diffusivity
  - Over- and undershooting
  - Stabilization needed!

- Solution: entropy viscosity method (Guermond et al., 2011)
  - Add artificial diffusion, but only in regions with high temperature/ compositional gradients



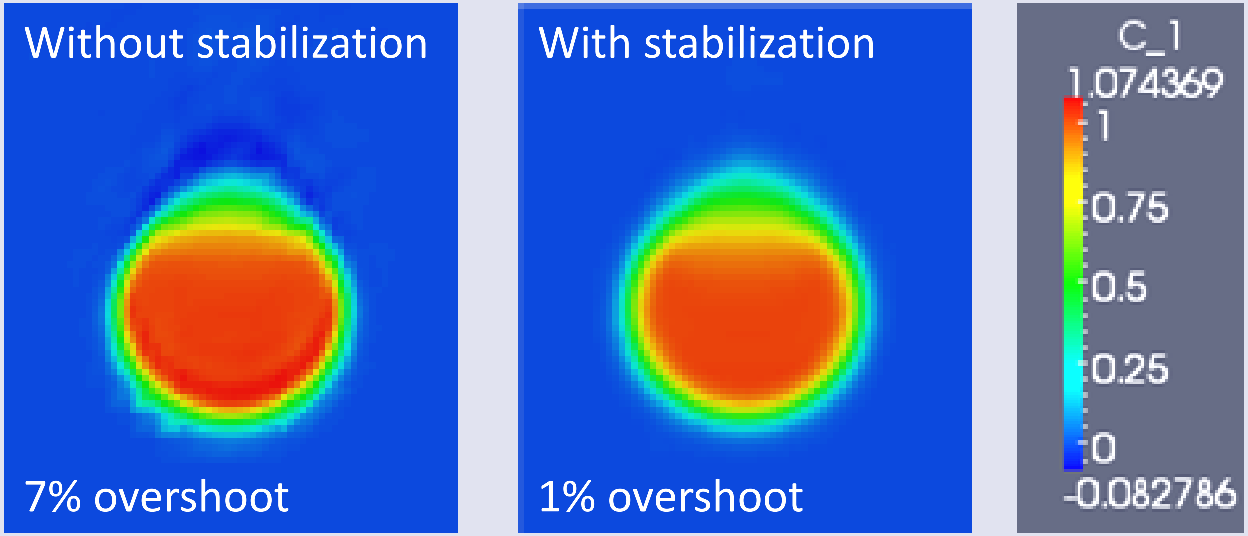
(Lenardic, Kaula, 1993)

Discretization

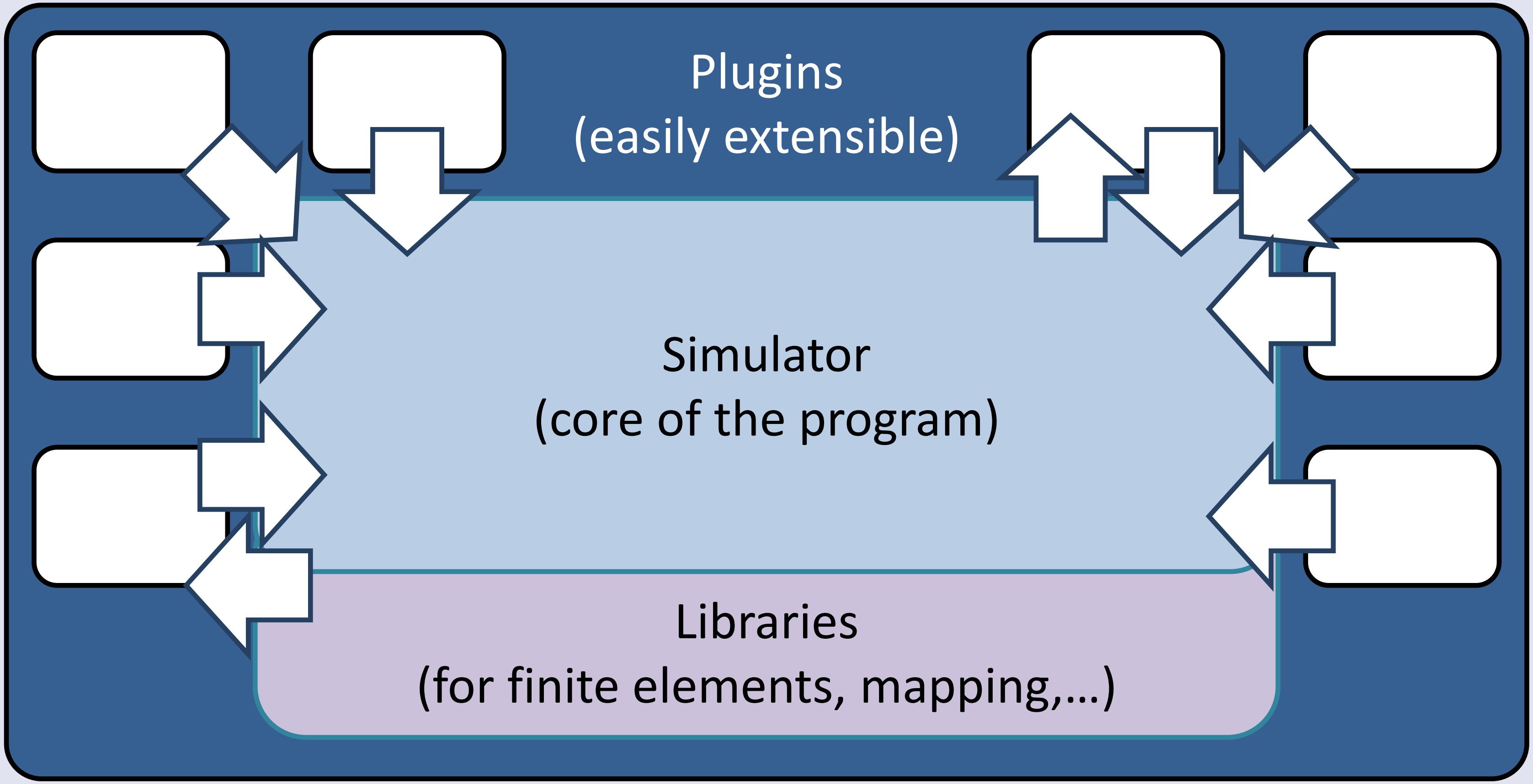
- Modified temperature/composition equation:

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T - \nabla \cdot (\kappa + \nu_h(T)) \nabla T = \gamma$$

- Result:

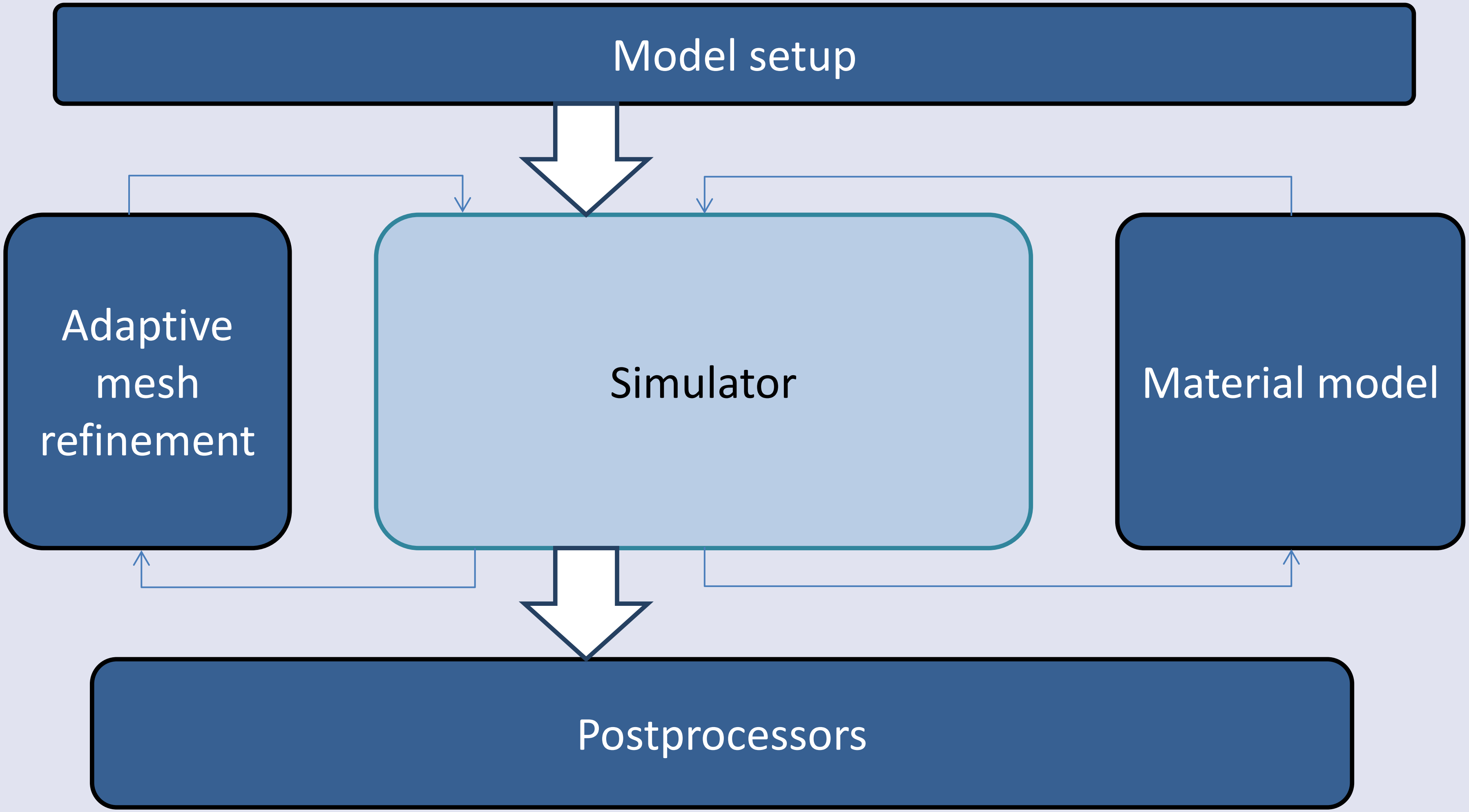


Modularity

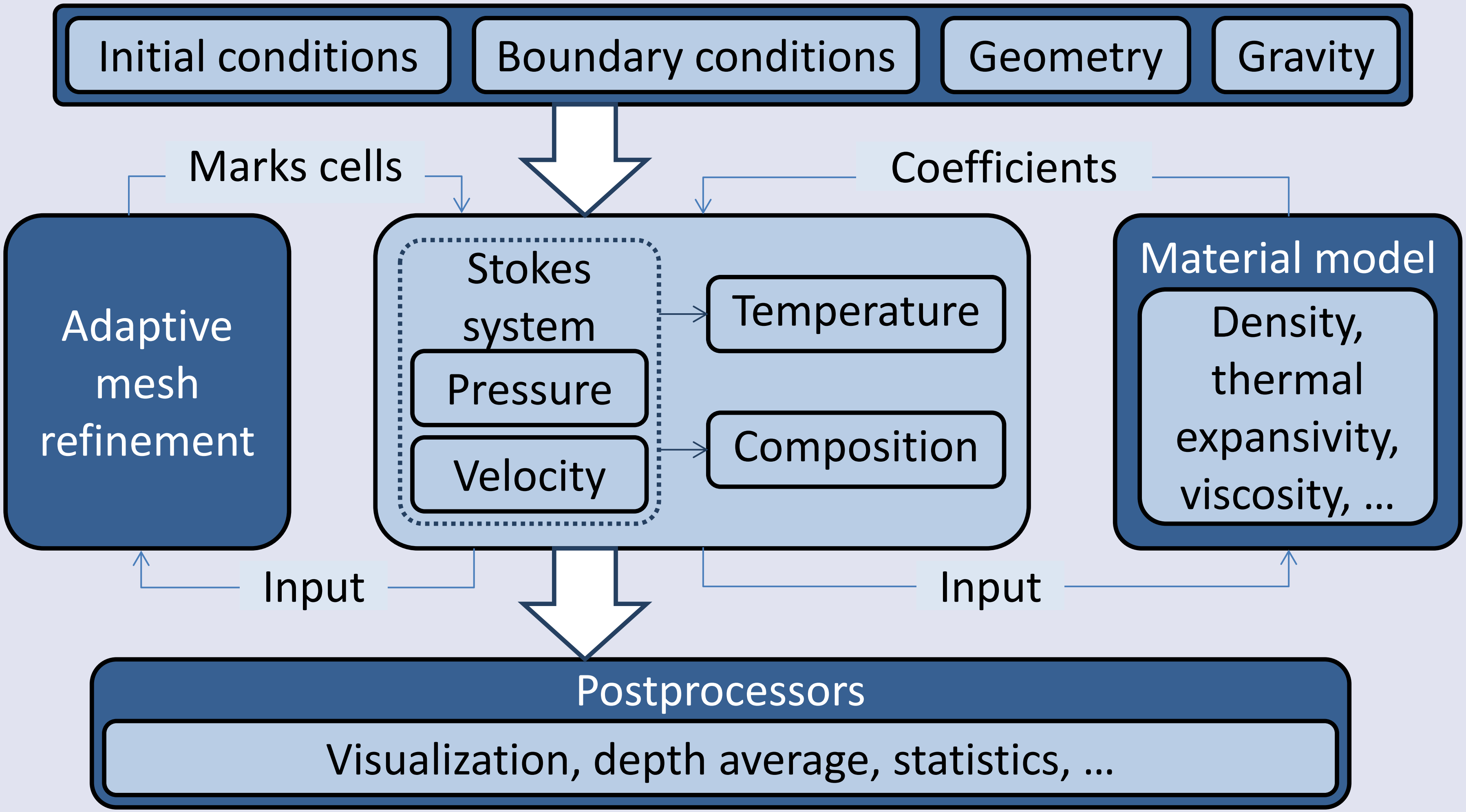


Plugins
(easily extensible)
Simulator
(core of the program)
Libraries
(for finite elements, mapping,...)

Modularity


Model setup
Adaptive mesh refinement
Simulator
Material model
Postprocessors

Modularity


Initial conditions
Boundary conditions
Geometry
Gravity
Marks cells
Coefficients
Adaptive mesh refinement
Stokes system
Pressure
Velocity
Temperature
Composition
Material model
Density, thermal expansivity, viscosity, …
Input
Input
Postprocessors
Visualization, depth average, statistics, …

Checkpointing

- After crash of program
- Use the final state of one model as initial condition for a series of models

→ Restart required

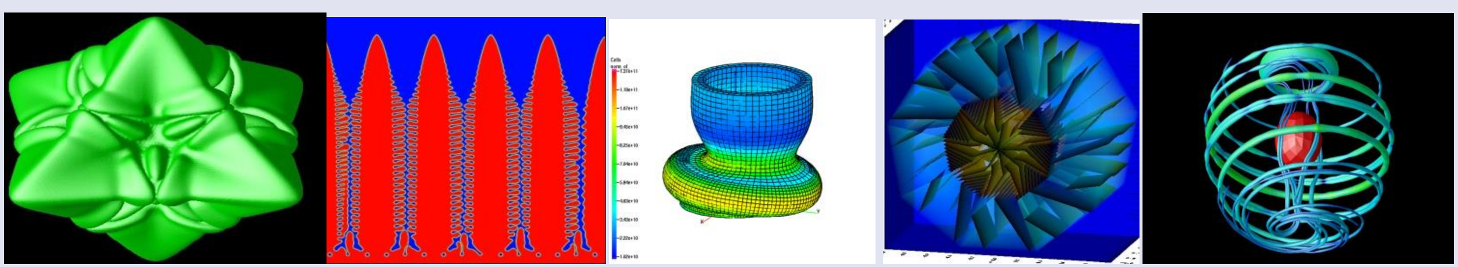
- Aspect creates checkpoint files
- Possibility to change parameters in restarted model (material laws, postprocessors)

Building on libraries

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

deal.II

- Meshes, finite elements, discretization: http://www.dealii.org/
- a C++ program library targeted at the computational solution of PDEs using adaptive finite elements

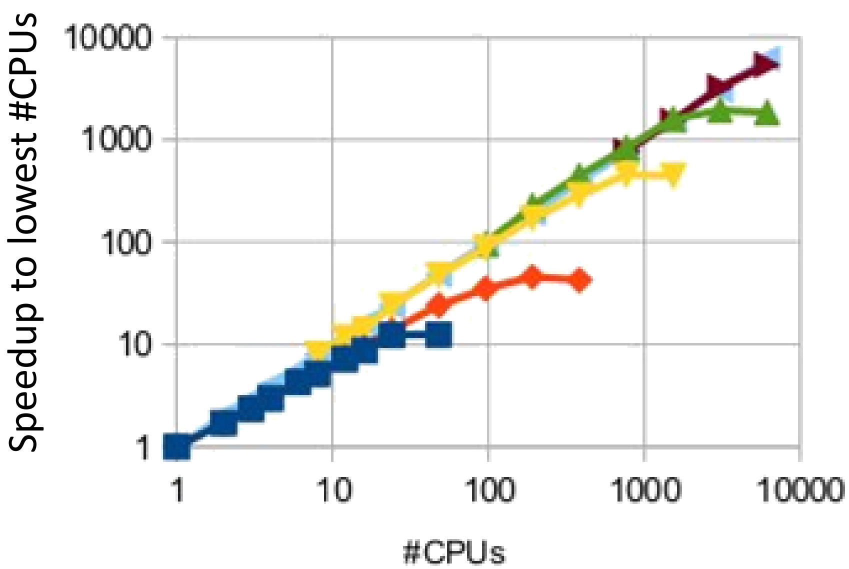


Efficient solvers

- Temperature: Conjugate gradient with preconditioner (LU decomposition)
- Stokes system (pressure & velocity): Generalized minimal residual method with preconditioner (includes conjugate gradient solves & algebraic multigrid)

Scaling

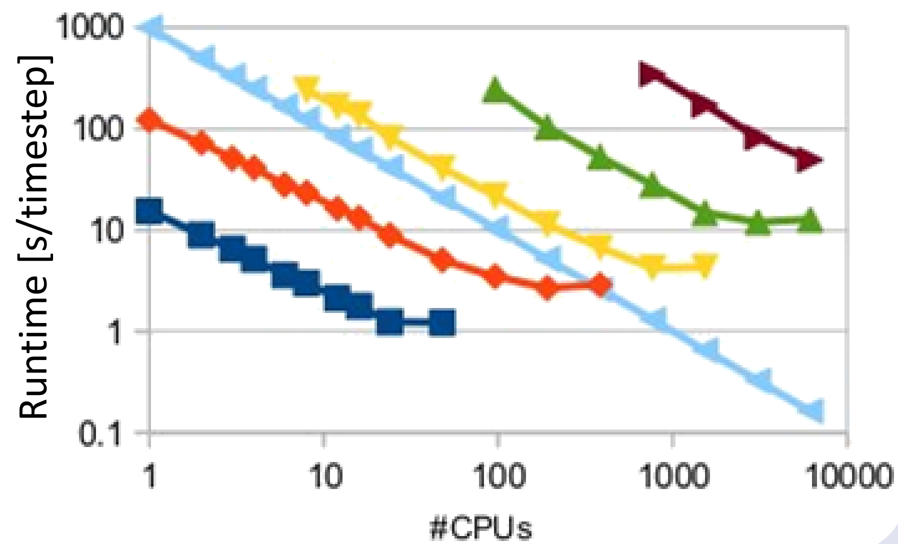
Speedup to maximal #DOFs/CPU



#DOFs

- 8.5e4
- 6.4e5
- 5.0e6
- 3.9e7
- 3.1e8
- Optimal

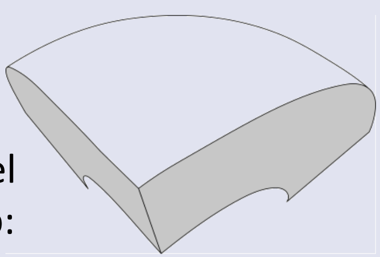
Strong Scaling



Resolution in km

- 360
- 180
- 90
- 45
- 22
- Optimal

Model Setup:



Work with R. Gassmoeller

Tutorial I
Convection in a 2D Box

(Nusselt-Rayleigh Relationship)

Nusselt-Rayleigh Relationship

- We will use ASPECT to study the relationship between the Rayleigh number and the surface heat flux
- In geodynamics, the Rayleigh number indicates the presence and strength of convection in the mantle
- The Nusselt number is the ratio of convective to conductive heat transfer
- If the Rayleigh number goes up, how does the Nusselt number change?
- How does the mesh resolution affect the accuracy of these results?

Nusselt-Rayleigh Relationship

1. Other output is shown in “output/statistics”. Open this file and see what sort of values are stored here.

   ```
   gedit output/statistics
   ```

2. We want to see how heat flux changes over time. Plot the results in gnuplot showing simulation time vs. heat flux

   ```
   gnuplot
   plot “output/statistics” using 2:20 with lines
   ```

3. What is the surface heat flux at the end of this run?

Nusselt-Rayleigh Relationship

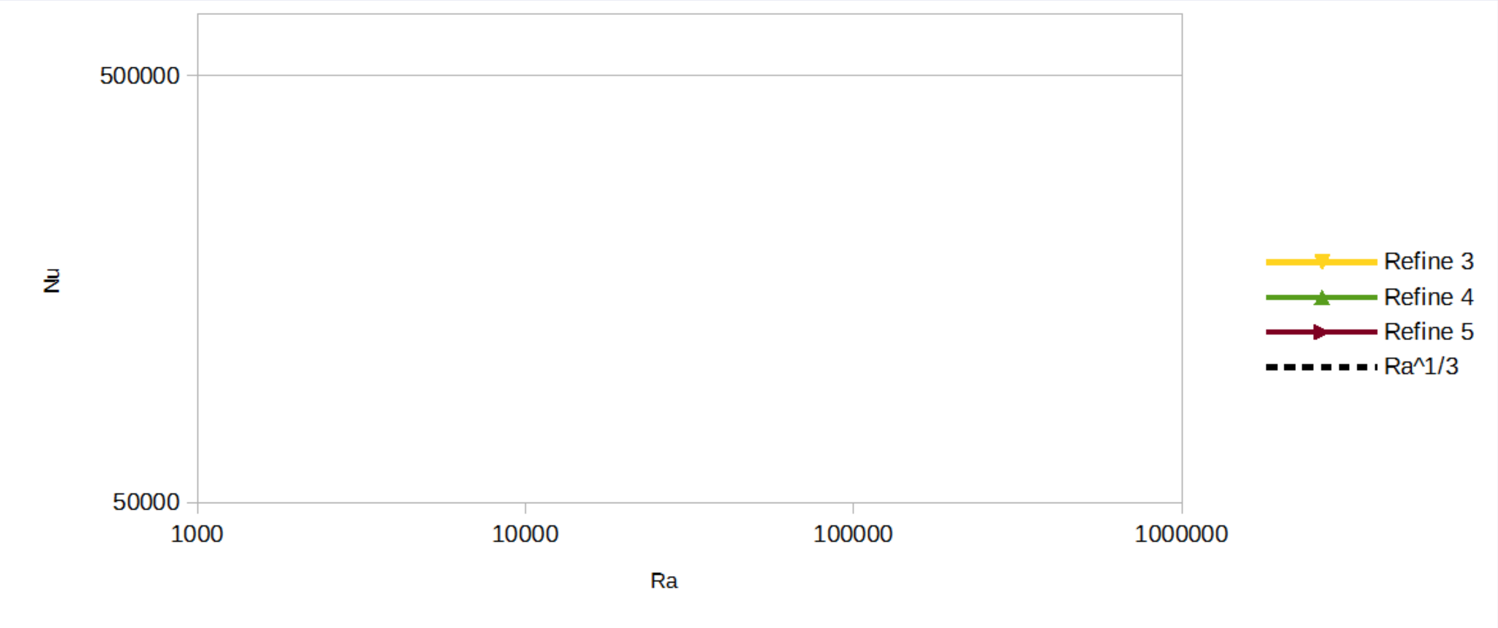
- We will split the class into multiple groups identified by the Rayleigh number, mesh refinement combination.
- You will need to:
  1. Modify the tutorial.prm file to use your assigned refinement, end time, and Rayleigh number

     Change the Rayleigh number by modifying the viscosity – remember, higher viscosity means lower Rayleigh number
  2. Run the simulation (`./aspect tutorial.prm`)
  3. Visualize the results and make sure they are realistic
  4. Report the heat flux number at the top boundary (boundary 3). This is related to the Nusselt number
  5. Note: to halt a simulation, press “Control-C”

Nusselt-Rayleigh Relationship

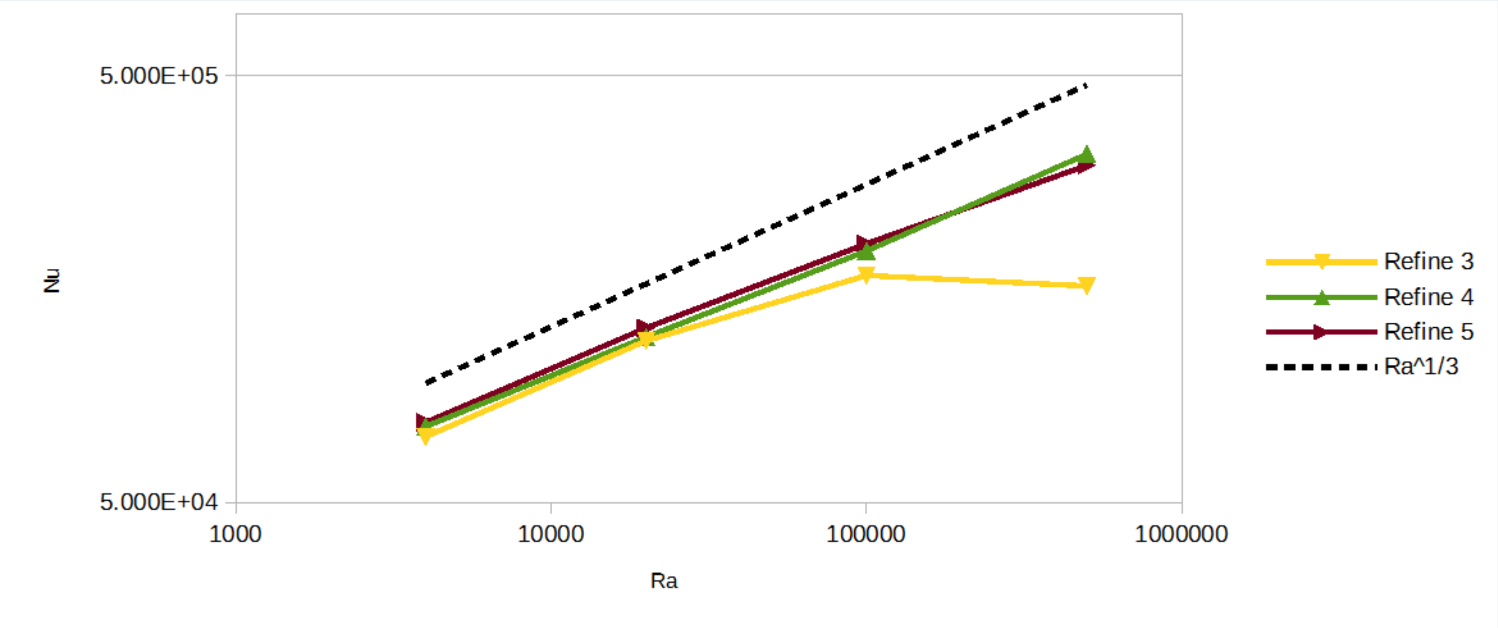
COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

Ra	4000	20000	100000	500000
end time	1.000E+12	2.000E+11	3.000E+10	5.000E+09
viscosity	1.275E+25	2.550E+24	5.099E+23	1.020E+23
Refine 3				
Refine 4				
Refine 5				
Ra^1/3				



Nusselt-Rayleigh Relationship

Ra	4000	20000	100000	500000
end time	1.000E+12	2.000E+11	3.000E+10	5.000E+09
viscosity	1.275E+25	2.550E+24	5.099E+23	1.020E+23
Refine 3	7.142E+04	1.198E+05	1.71E+005	1.61E+005
Refine 4	7.544E+04	1.222E+05	1.945E+05	3.278E+05
Refine 5	7.719E+04	1.284E+05	2.023E+05	3.086E+05
Ra^1/3	9.524E+04	1.629E+05	2.785E+05	4.762E+05



Things to play with

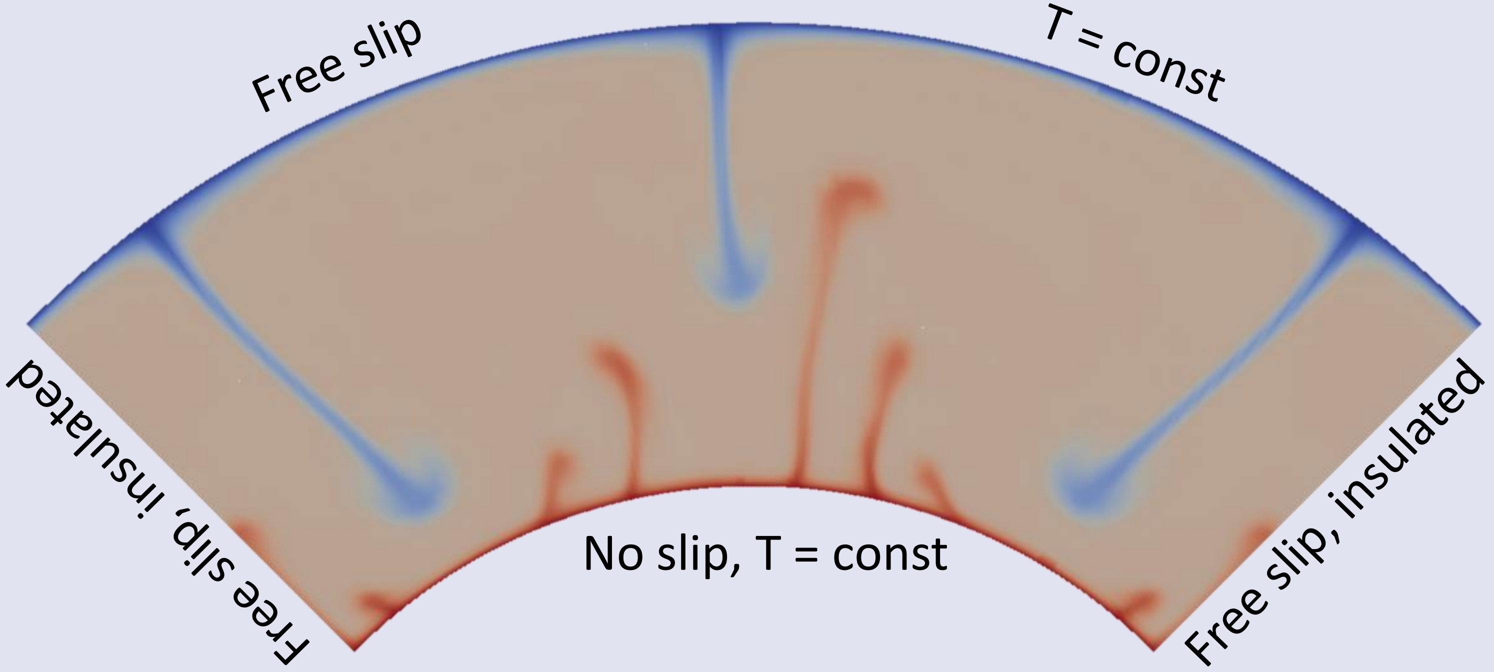
- Plot Nusselt number over time
- Change geometry
- Change boundary conditions
- Open manual and go through the list of cookbooks
  input files are in `~/aspect-source/cookbooks`

Tutorial II
Using the adaptive mesh refinement & spherical shell geometry

Overview

- At the end of this tutorial, you should be able to:
  - Set up a model with Earth-like geometry and temperature in Aspect
  - Set up a model with adaptive mesh in Aspect
  - Decide which mesh refinement strategy to use
  - Know a bit more about how the mesh influences the flow field ☺

Setup: Convection in a Shell



- Geometry: Quarter of a spherical shell
- Constant initial temperature with a perturbation to start the upwelling

Tasks

- We will split the class into multiple groups identified by the mesh refinement (number of global refinements)
- You will need to:
  1. Modify the spherical_shell.prm file to use your assigned refinement number/strategy
  2. Run the simulation
  3. Visualize the results and make sure they are realistic
  4. Check which features of the flow field are resolved
  5. Note: to halt a simulation, press “Control-C”

Using ASPECT

- Edit the input file:

1. Change to the appropriate directory

```
cd ~/Desktop
```

2. Open the parameter file for editing

```
gedit spherical_shell.prm
```

Mesh refinement

```
subsection Mesh refinement
  set Initial global refinement                = 5
  set Initial adaptive refinement              = 0
  set Strategy                                 = temperature
  set Time steps between mesh refinement = 0
  set Coarsening fraction                      = 0.0
  set Refinement fraction                      = 0.0
end
```

This is what we want to change:

- Group 1: 3
- Group 2: 4
- Group 3: 5

Running the model

```
./aspect spherical_shell.prm
```

Or in parallel

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

Material model

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

```
set Adiabatic surface temperature      = 1600

subsection Material model
  set Model name = simple
  subsection Simple model
    set Thermal expansion coefficient = 2e-5
    set Viscosity                     = 3e21
    set Thermal viscosity exponent    = 3
    set Reference temperature         = 1600
  end
end
```

These should be the same

Temperature-dependent viscosity

Geometry & gravity model

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

```
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 earth-like
end
```

The gravity model has to be changed together with the geometry

Initial conditions

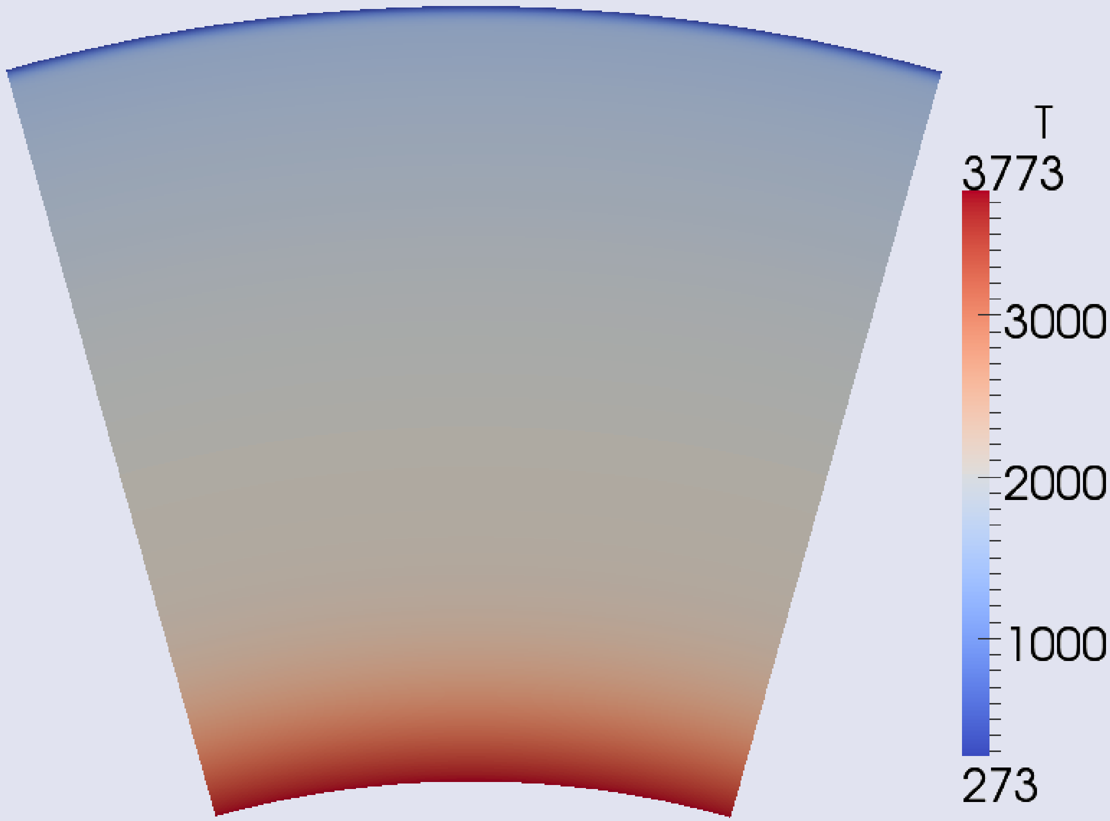
```
set Adiabatic surface temperature     = 1600
```

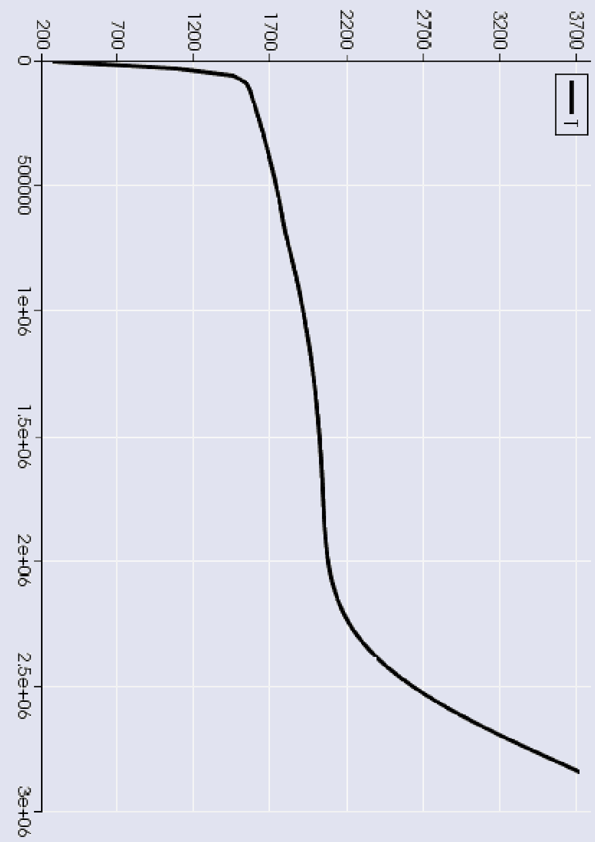
```
subsection Initial conditions
  set Model name = adiabatic

  subsection Adiabatic
    set Amplitude = 10
    set Radius = 500000
  end
end
```

This is the temperature used as initial condition

Adiabatic initial conditions

- Calculated using depth-dependent ρ, α, c_p





Boundary conditions

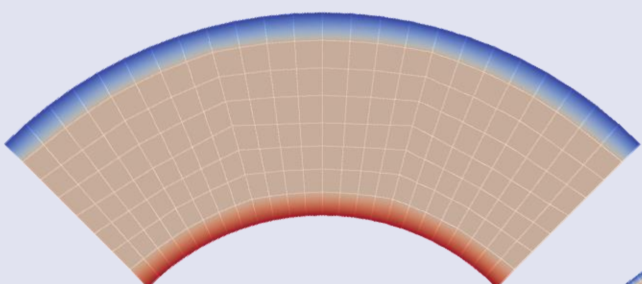
```
subsection Model settings
  set Zero velocity boundary indicators       = 0
  set Tangential velocity boundary indicators = 1, 2, 3
  set Prescribed velocity boundary indicators =
  set Fixed temperature boundary indicators   = 0, 1

  set Include shear heating                   = false
  set Include adiabatic heating               = false
end
```

Boundary conditions

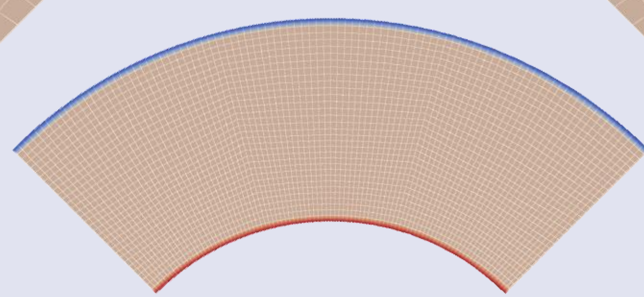
```
subsection Model settings
  set Zero velocity boundary indicators       = inner
  set Tangential velocity boundary indicators = outer, left,
   right
  set Prescribed velocity boundary indicators =
  set Fixed temperature boundary indicators   = inner, outer

  set Include shear heating                   = false
  set Include adiabatic heating               = false
end
```

Mesh refinement

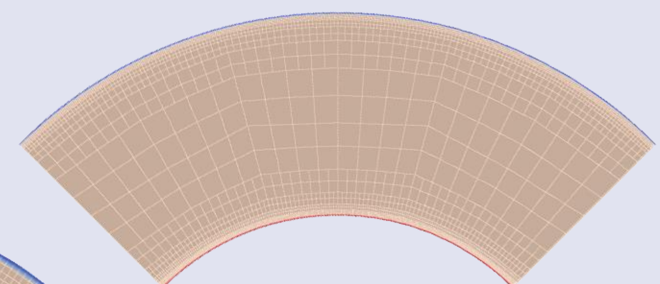
```
subsection Mesh refinement
  set Initial global refinement                = 5
  set Initial adaptive refinement              = 0
  set Strategy                                 = temperature
  set Time steps between mesh refinement       = 0
  set Coarsening fraction                      = 0.05
  set Refinement fraction                      = 0.3
end
```



Global refinement = 3



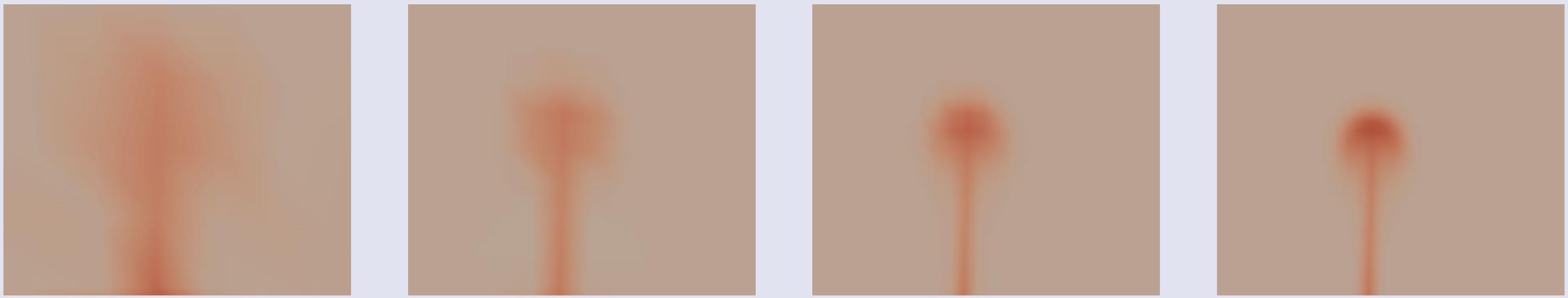
Global refinement = 5



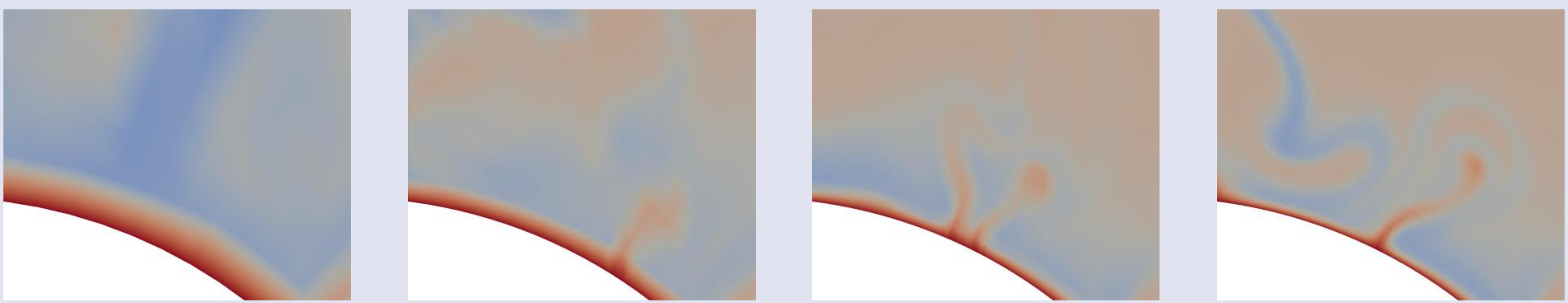
Global refinement = 4
Adaptive refinement = 2

Results

Time snapshots of models with different resolution



Group 1: 3	Group 2: 4	Group 3: 5	Group 4: 6



Mesh refinement

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

```
subsection Mesh refinement
  set Initial global refinement                = 5
  set Initial adaptive refinement              = 0
  set Strategy                                 = temperature
  set Time steps between mesh refinement = 5
  set Coarsening fraction                      = 0.05
  set Refinement fraction                      = 0.3
end
```

This is what we want to change:

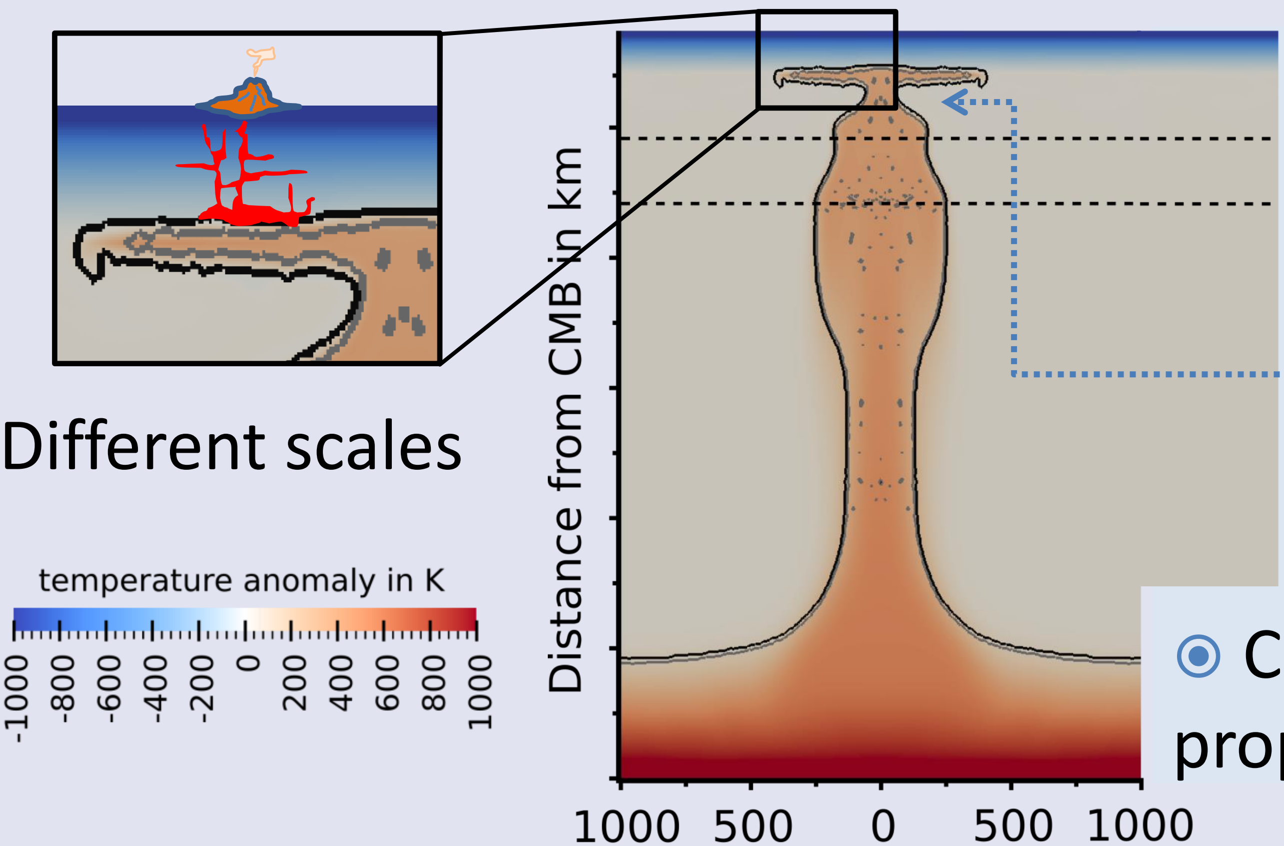
- Group 1: 4 + 0
- Group 2: 5 + 0
- Group 3: 6 + 0

Set to a value > 0 to enable adaptive refinement

Running

```
./aspect spherical_shell.prm
```

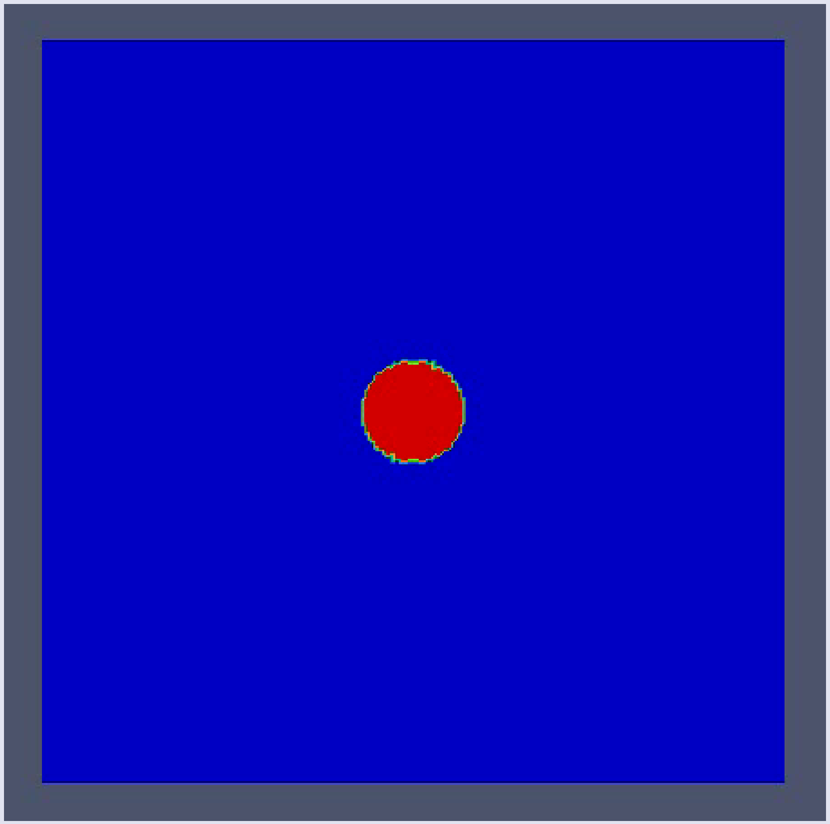
Numerical Challenges



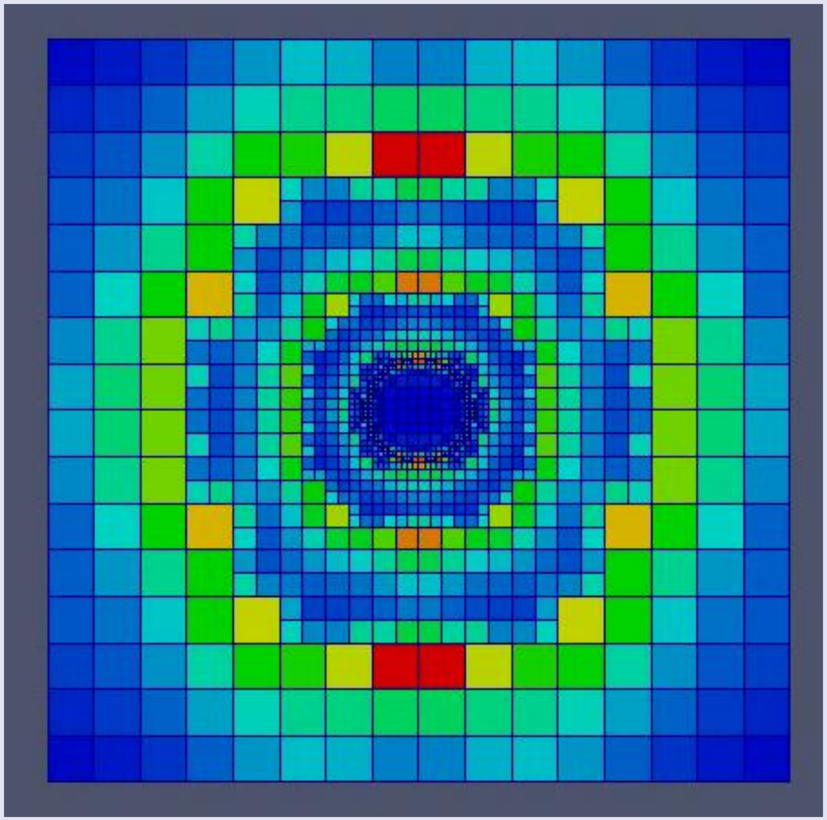
- High viscosity contrasts
- Advection of steep thermal/ compositional gradients
- Complex material properties
- Problems with large number of DOFs

Mesh adaptation

- Example: Composition as refinement strategy



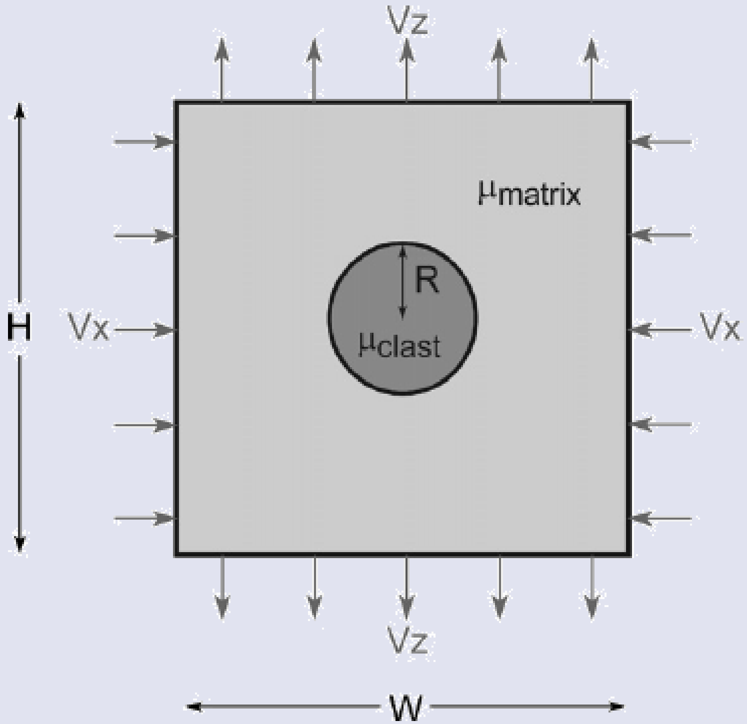
Compositional field



Mesh cells, colors indicate the estimated error

Mesh adaptation

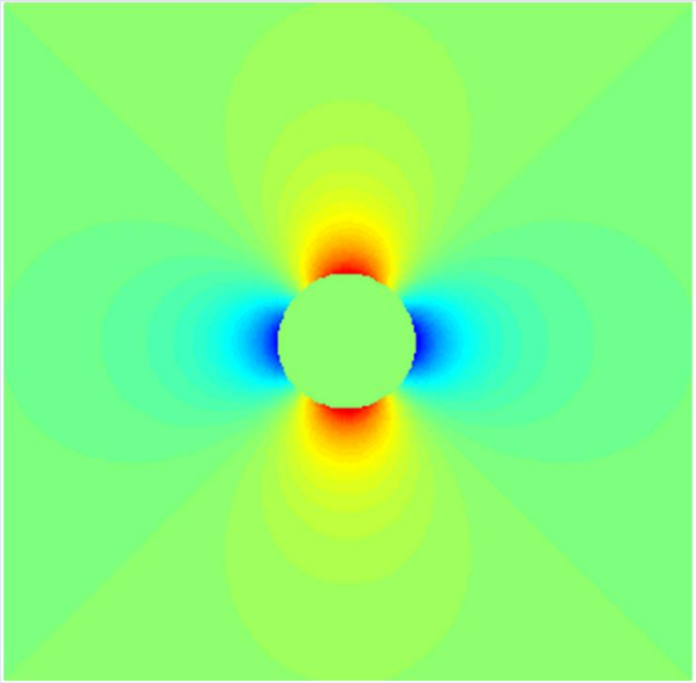
- Stokes solver for problems with complex interfaces and high viscosity ratios



Circular inclusion test, viscosity constrast 10^3

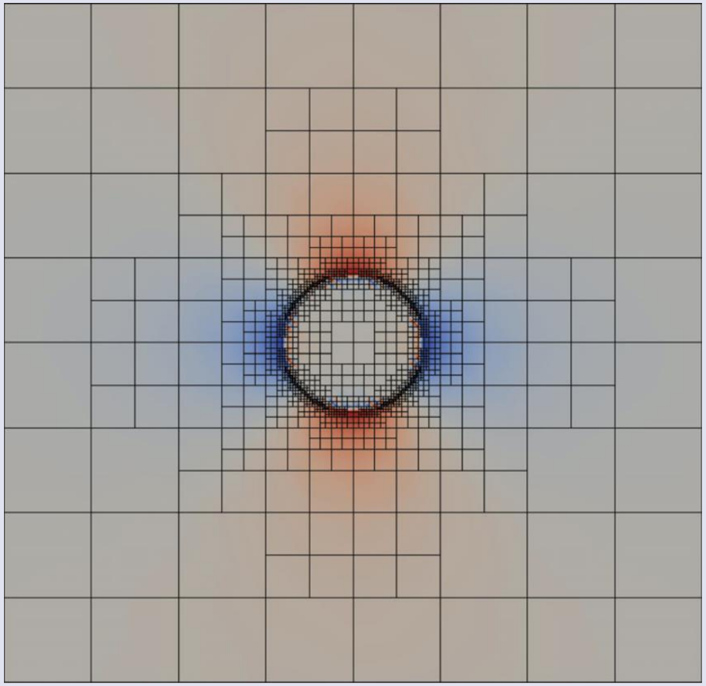
Mesh adaptation

Analytical Solution for Pressure:



(Schmid, Podladchikov, 2003)

Aspect's solution for Pressure:



Mesh adaptation

Choose **Strategies**: *temperature, density, velocity, composition, thermal energy density*

Calculate error estimate c_K (based on 2nd derivatives & cell diameter)

$$E = \sum_{K \in T} c_K$$

Total error estimate E

Normalize refinement criteria?

Scale errors for each criterium?

Add errors/take maximum?

Choose **refinement + coarsening fraction** a

Look for the smallest subset M

$$aE = \sum_{K \in M} c_K$$

(sum up c_K in the cells with the largest/smallest error until you reach fraction a of the error)

Mark those cells for refinement/coarsening

Mesh refinement options

- Strategies: (nonadiabatic) temperature /pressure, composition, density, velocity, viscosity, thermal energy density…
- Refinement criteria scaling factors
- min/max refinement level function
  - Phase transitions / jump in material properties
- Additional refinement times
  - Onset of new processes (convection? melting? plate velocities?)

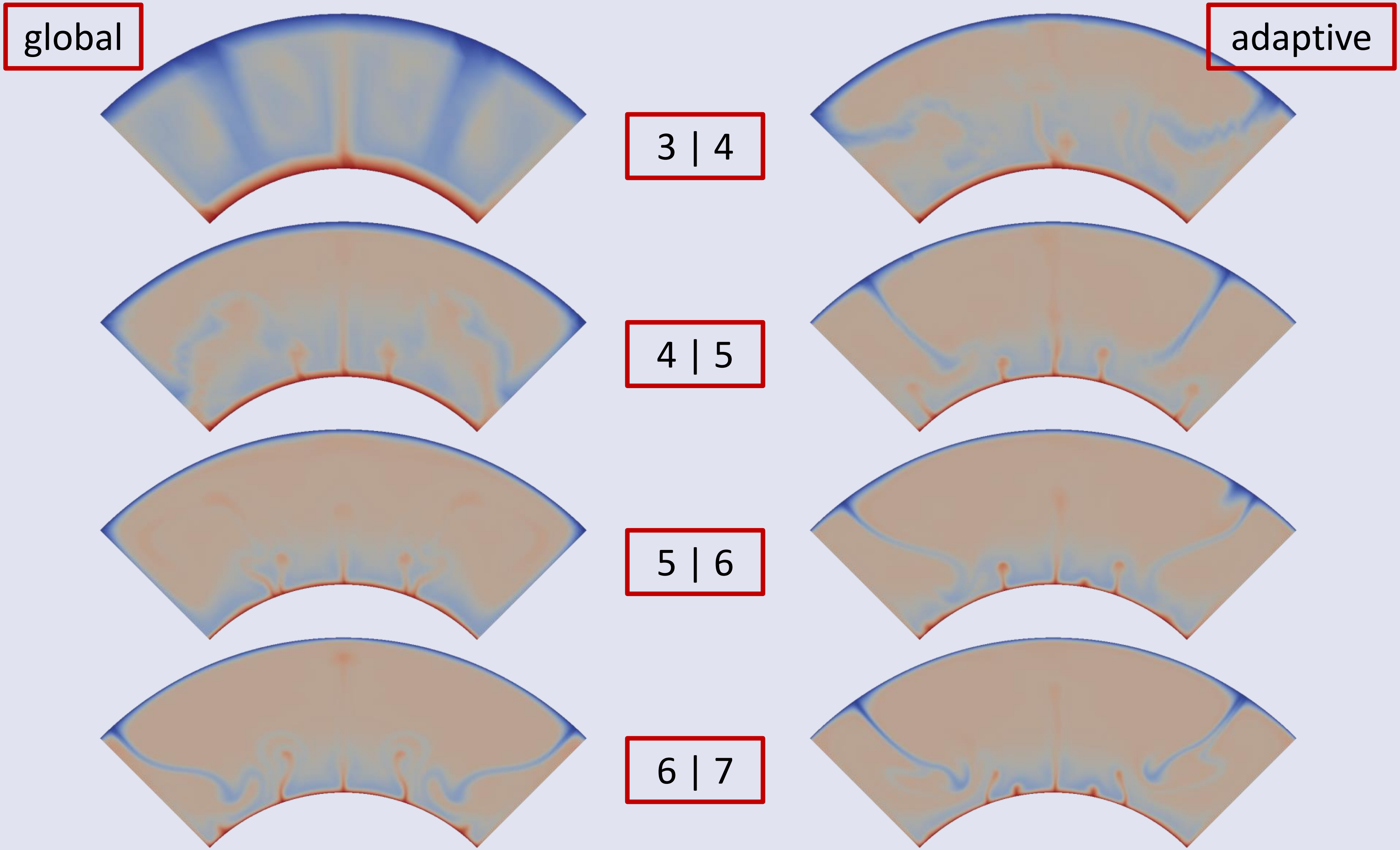
Inspecting the results

1. With Paraview

```
paraview
```

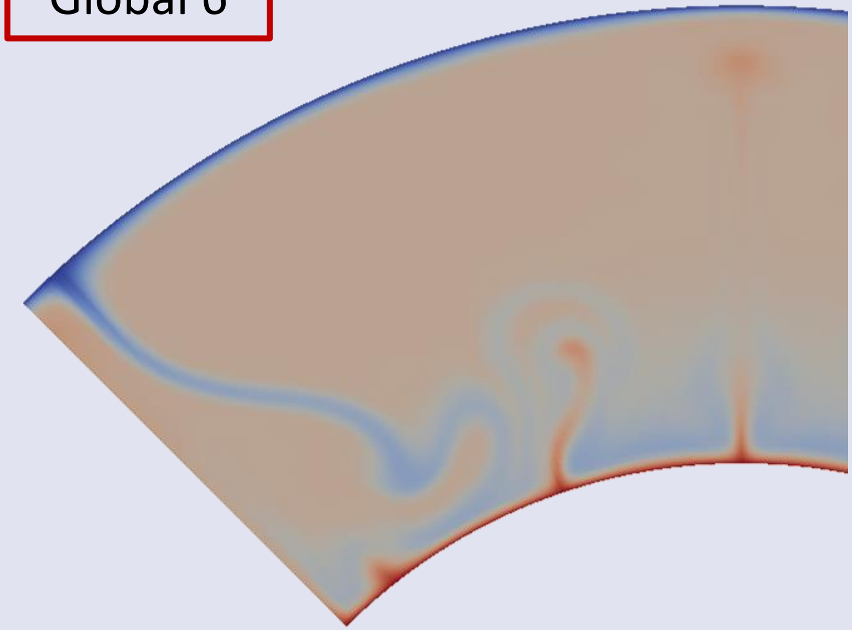
2. How does the flow field change with varying the resolution?
3. How does the runtime change with the adaptive refinement compared to global refinement?
4. What refinement / coarsening fraction is sufficient?

Results

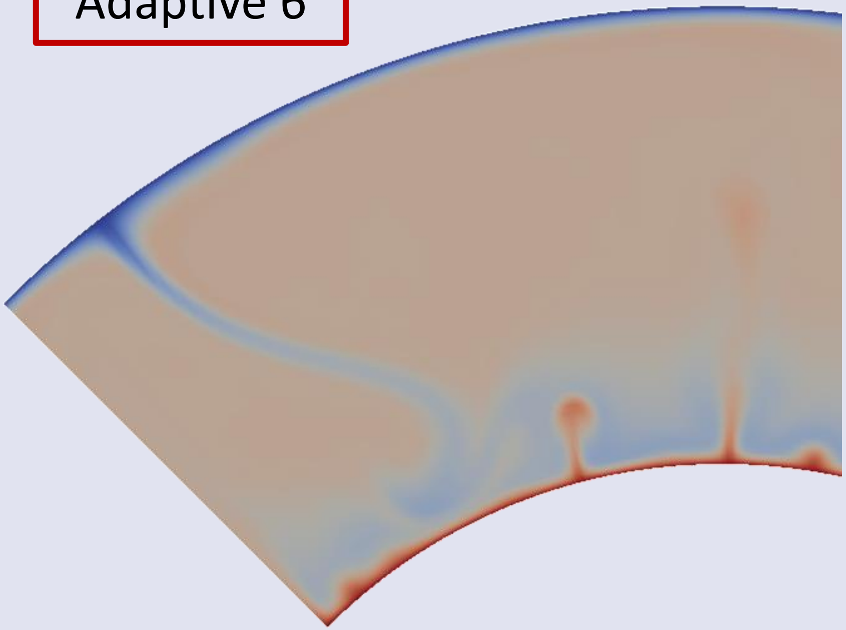


Results

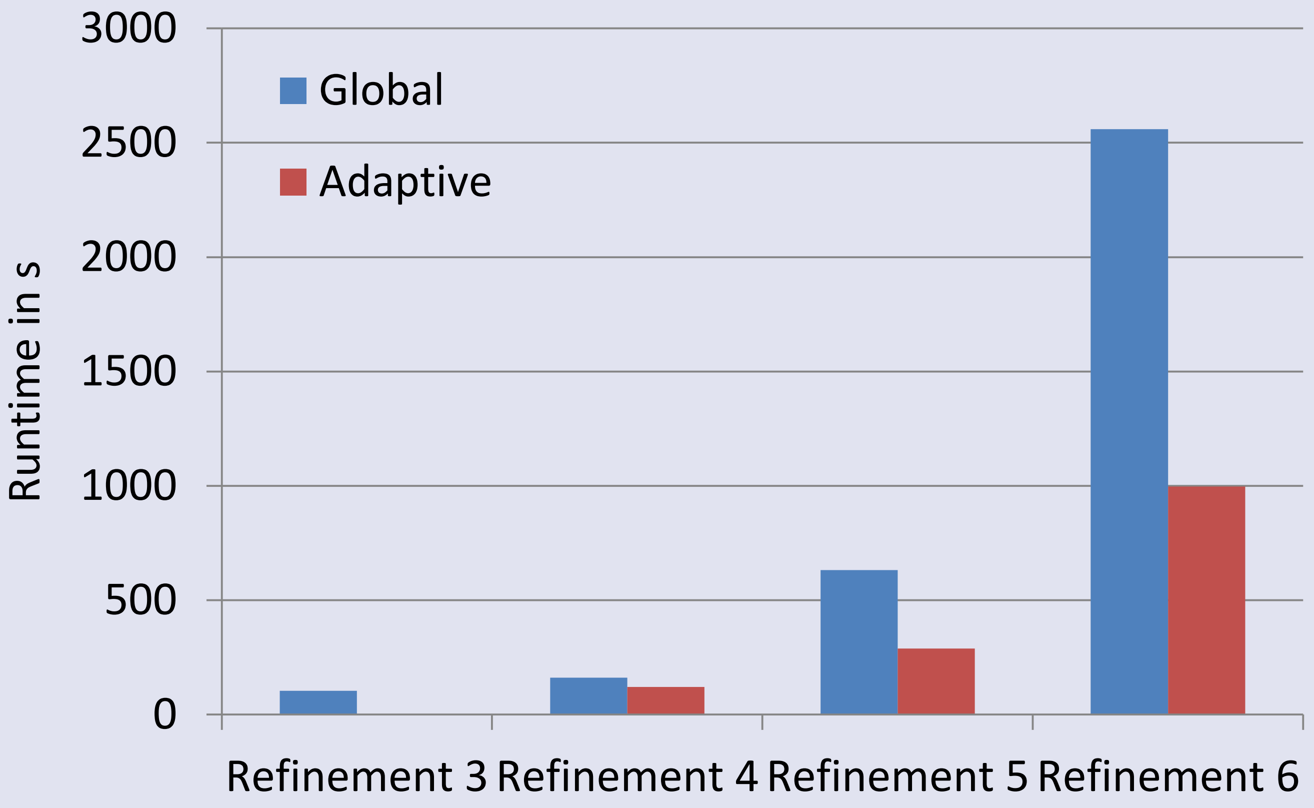
Global 6



Adaptive 6



Results



3000
2500
2000
1500
1000
500
0
Runtime in s
Global
Adaptive
Refinement 3
Refinement 4
Refinement 5
Refinement 6

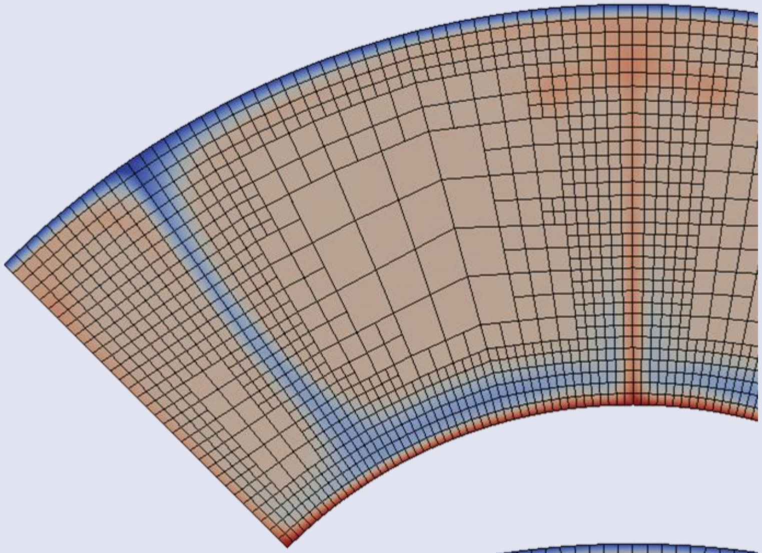
Mesh refinement

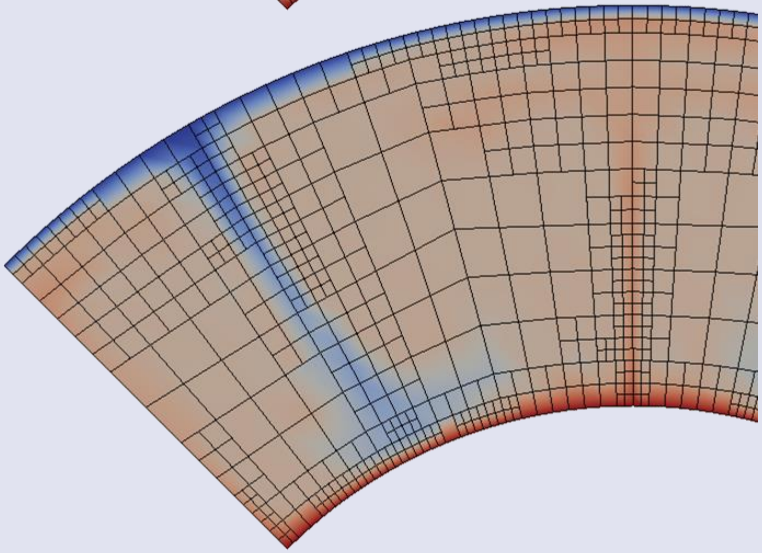
```
subsection Mesh refinement
  set Initial global refinement              = 4
  set Initial adaptive refinement            = 2
  set Strategy                               = temperature
  set Time steps between mesh refinement     = 5
  set Refinement fraction                    = 0.3
  set Coarsening fraction                    = 0.05
end
```

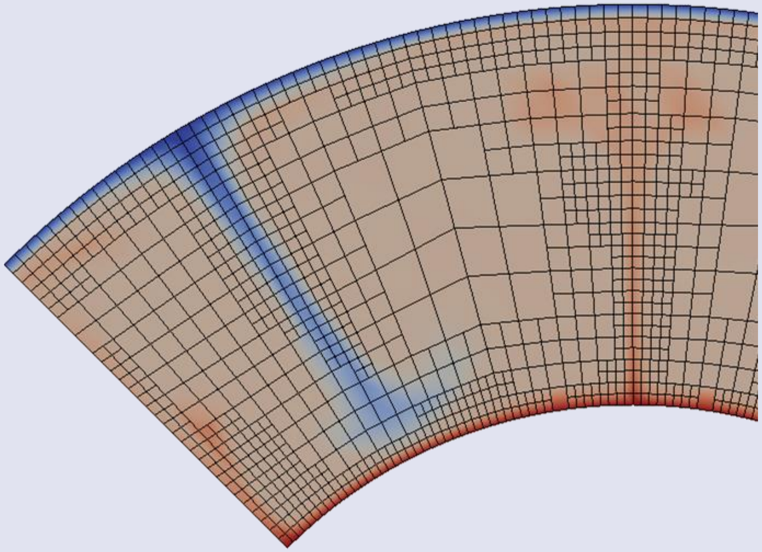
This is what we want to change:

- Group 1: 0.6 + 0.01
- Group 2: 0.1 + 0.1

Results







Things to play with

- Plot Nusselt number over time
- Change geometry
- Change boundary conditions
- Open manual and go through the list of cookbooks
  input files are in `~/aspect-source/cookbooks`