ASPECT

Introduction – Tutorial – Applications

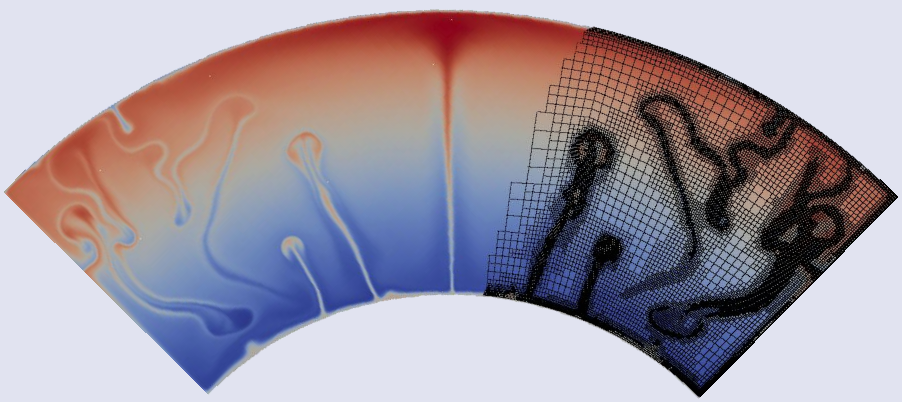
Blockkurs Fortgeschrittene Geodynamik
08.03.2016

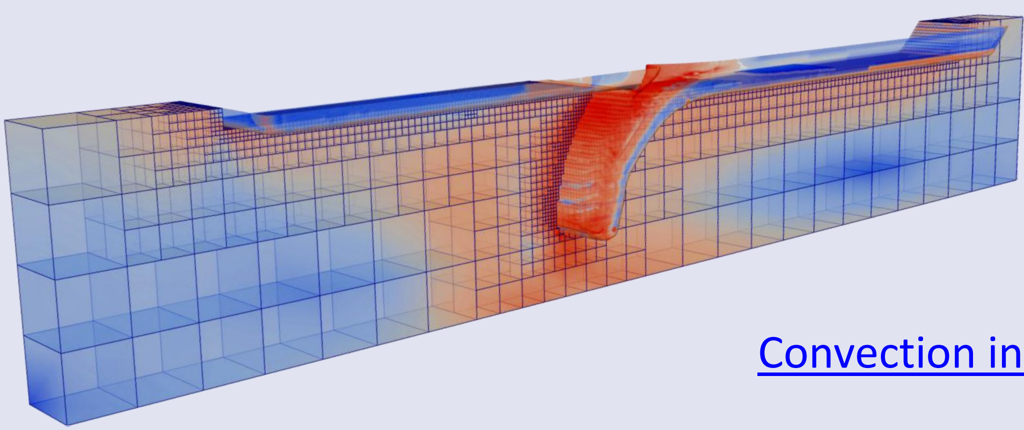
Anthony Osei Tutu (GFZ, Sektion 2.5)
Eva Bredow (GFZ, Sektion 2.5)

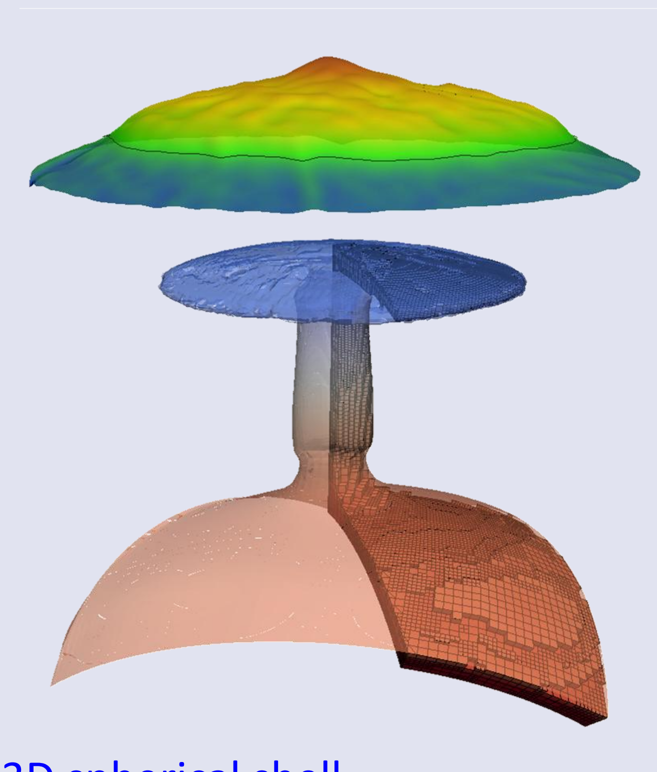
What is Aspect?

ASPECT

- Advanced Solver for Problems in Earth's ConvecTion -







[Convection in a 3D spherical shell]

Codes in Geodynamics

- Some widely used codes
- Almost no codes use adaptively refined meshes
- Almost all codes use lower order elements
- Most codes use “simple” solvers
- No code has been “designed” with a view to
  – extensibility
  – maintainability
  – correctness

Geodynamics: Design challenges

CIG COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

Requirements as “community code”:

- solve problems of interest (to geodynamicists)
- well tested
- modern numerical methods
- easy to extend
- freely available = open code

Numerical methods

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

- 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 the steps above
- Modularity of the code

Credits

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

Website and manual:

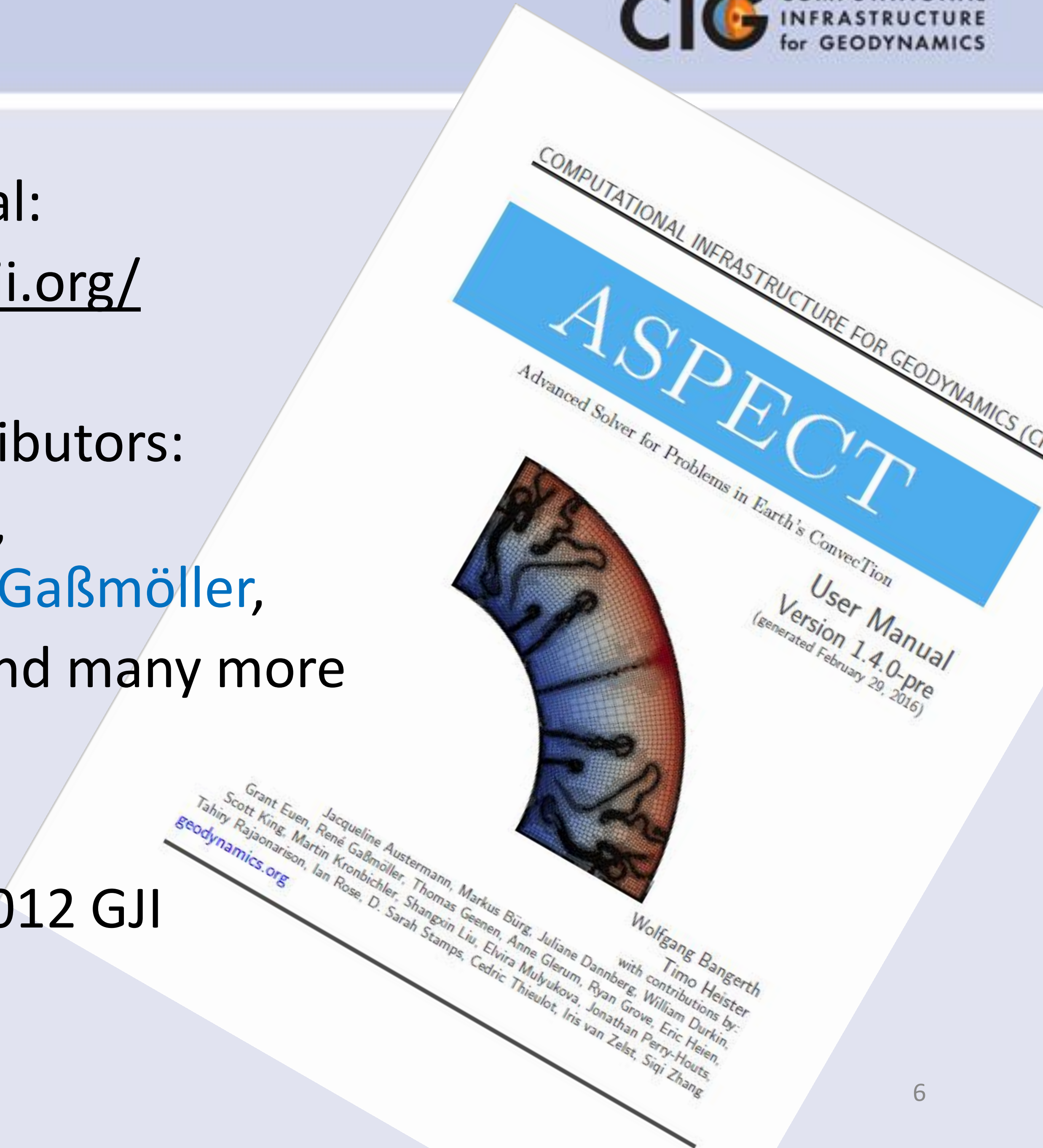
https://aspect.dealii.org/

Developers & contributors:

Wolfgang Bangerth,
Timo Heister, René Gaßmöller,
Juliane Dannberg and many more

Publication:

Kronbichler et al. 2012 GJI



Setup of the numerical model

- Model 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
- Look at the parameter file:
  cd ASPECT_TUTORIAL/models/

  gedit tutorial.prm

ASPECT - General

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

- General parameters:

Internal calculations use seconds, but output in years

2D problem

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

Simulation output will be stored in the directory named “output”

= 5×10^{10} years
= 50 billion years

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

Divergence of stress tensor

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

Pressure gradient

(Total pressure instead of only dynamic pressure)

Gravity force

$\mathbf{u}$	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

Includes compressibility

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} + \rho \cdot \mathrm{div}\, \vec{v} = 0$$

(with the assumption $\frac{\partial \rho}{\partial t} = 0$)

Mass change in a given volume

In- / outflux of mass

$\mathbf{u}$	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

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

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

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

Conservation of energy

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

Advection of compositional fields

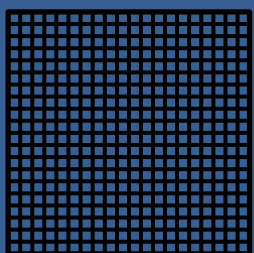
Field method (instead of tracer method)

Geometry model

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

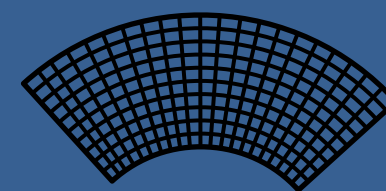
2D or 3D?

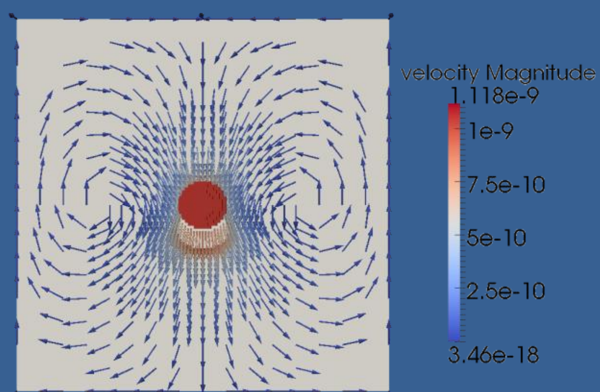
Geometry model

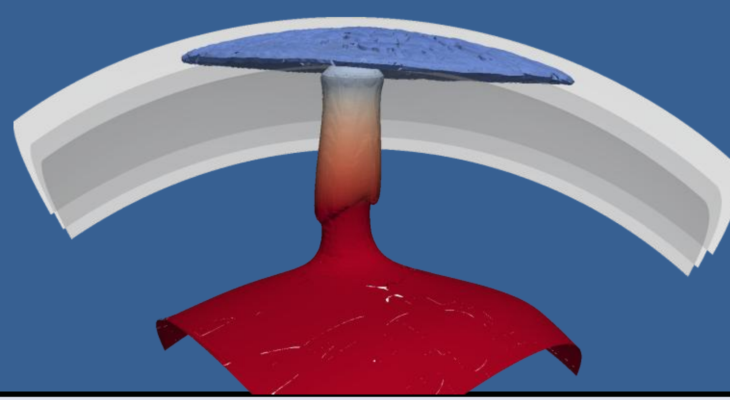


Box

Spherical shell

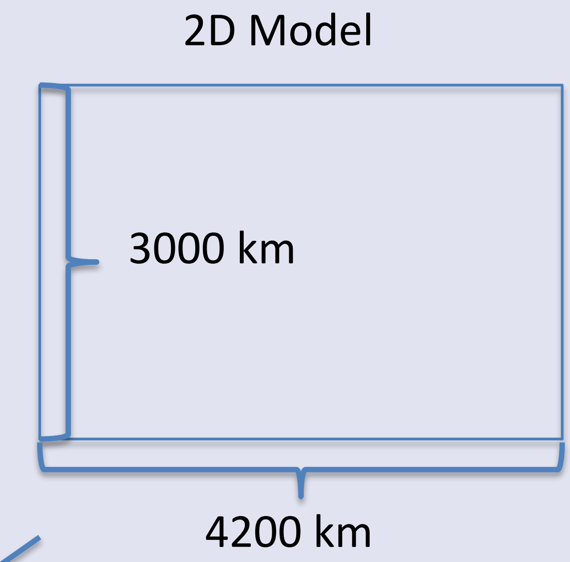






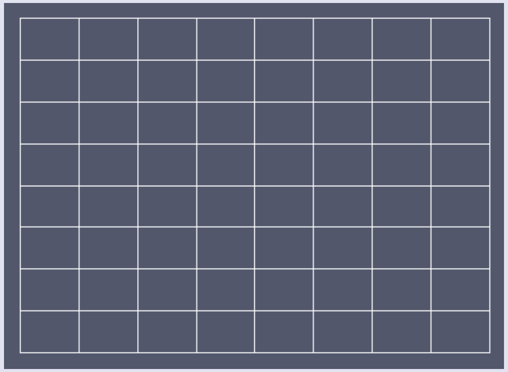
ASPECT - Geometry

- 2D box = rectangle,
  3D box = cuboid
- Depth of the box = 3×10^6 m
- Width of the box = 4.2×10^6 m
- Make sure that various units fit together!

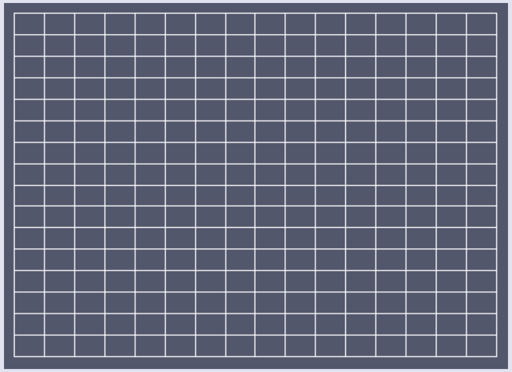



```
subsection Geometry model
        set Model name = box
        subsection Box
                set X extent = 4.2e6
                set Y extent = 3e6
        end
end
```

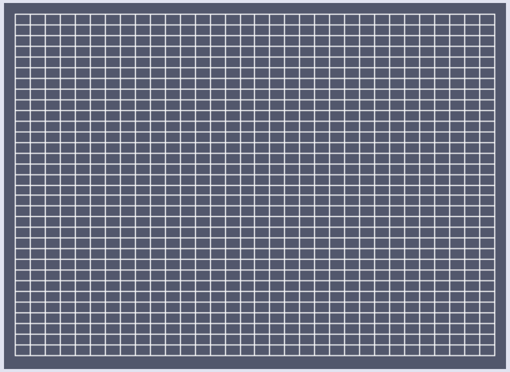
ASPECT - Discretization



REFINE=3 (8x8 cells)



REFINE=4 (16x16 cells)



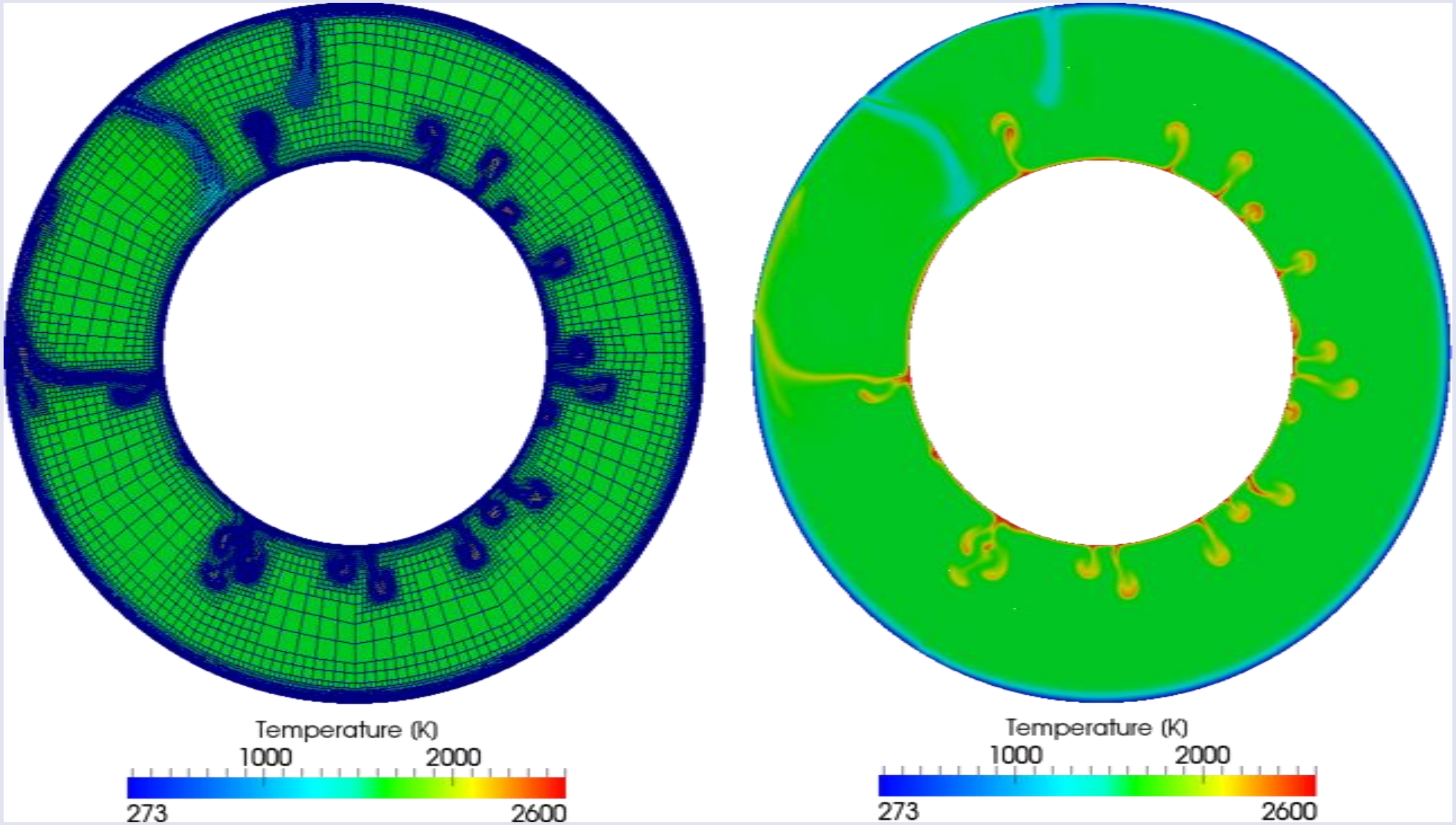
REFINE=5 (32x32 cells)

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

"grid spacing" of the mesh, for this tutorial: REFINE = 3 or 4 or 5

turned off → the mesh does not change during the simulation

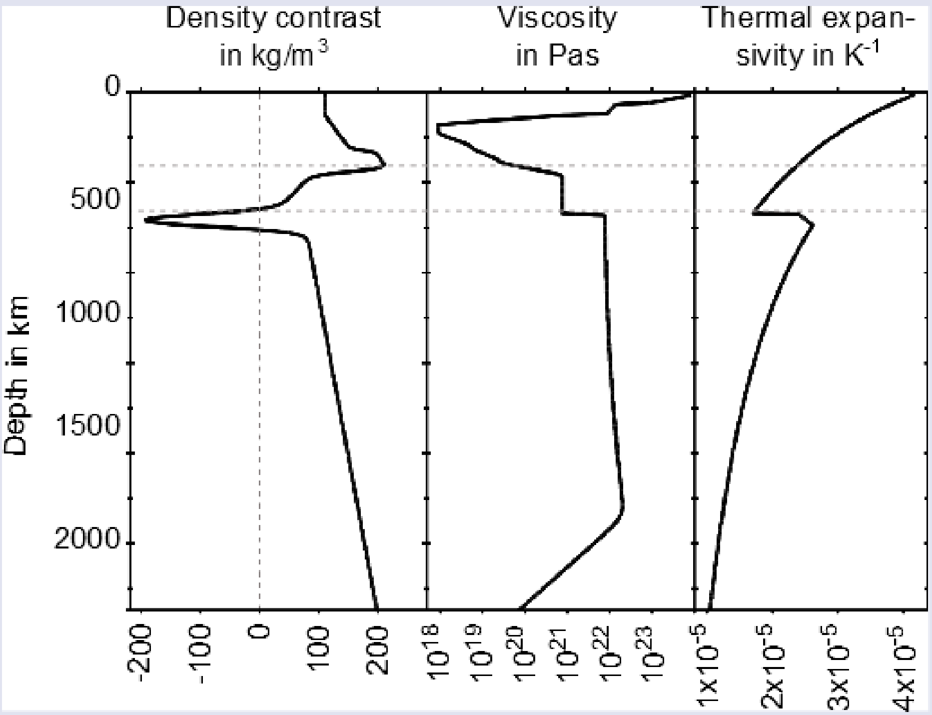
Mesh adaptation

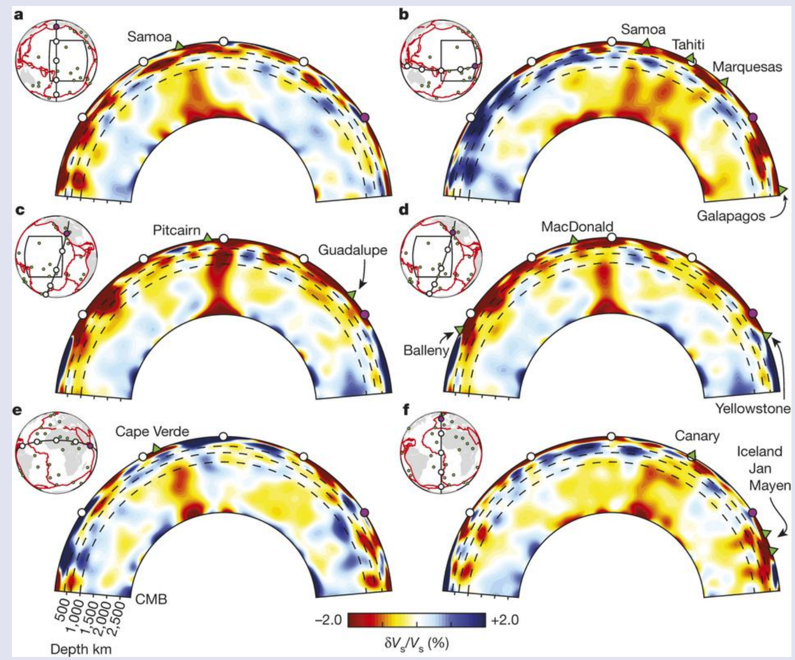


Material model

Input:

Temperature, pressure, composition, strain rate, position





Densities for example from seismic tomography velocities

ASPECT - Model Parameters

- Use a built in material model or implement your own
- Several parameters which control reference density, temperature dependence of viscosity, etc.

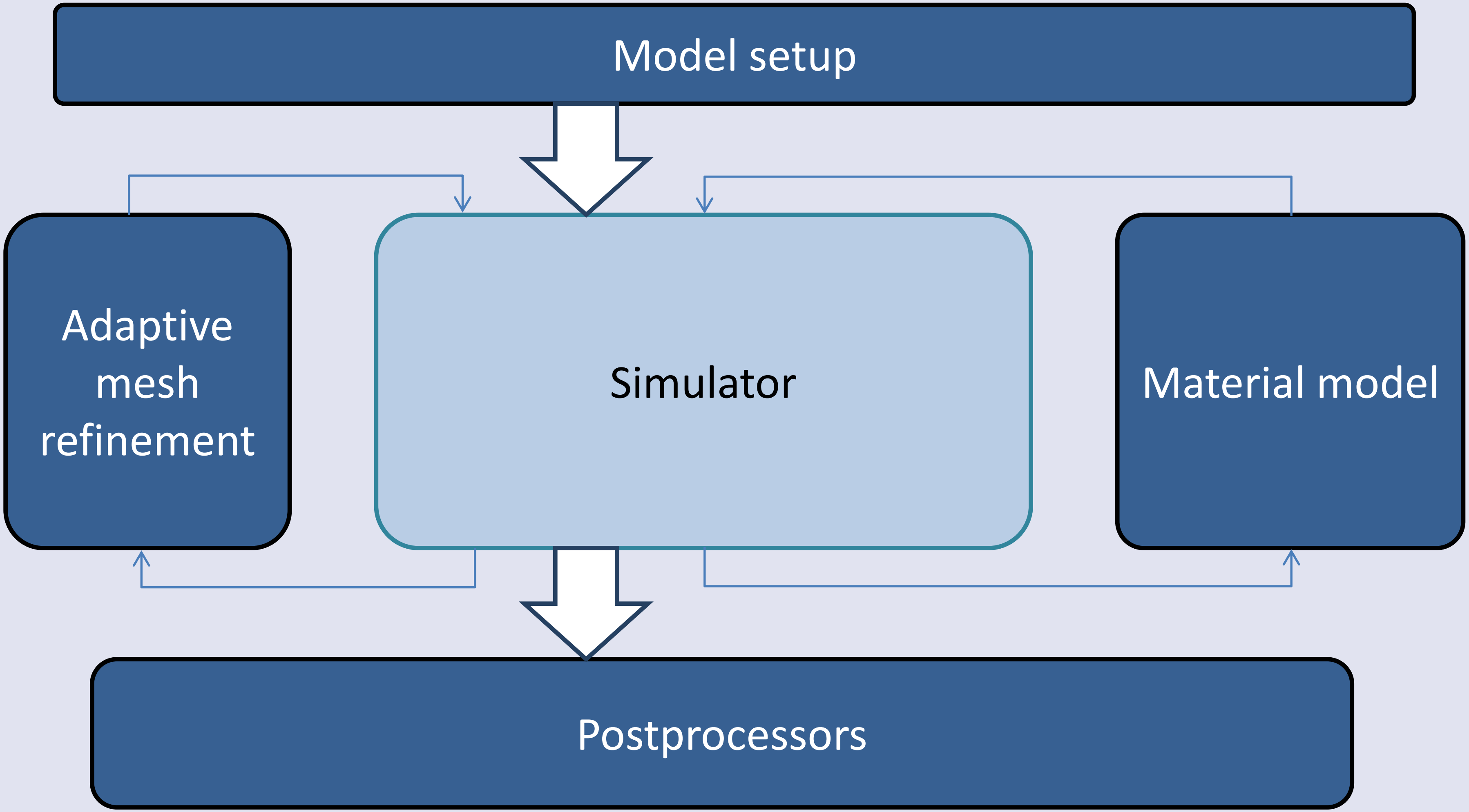
Default Values:

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

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

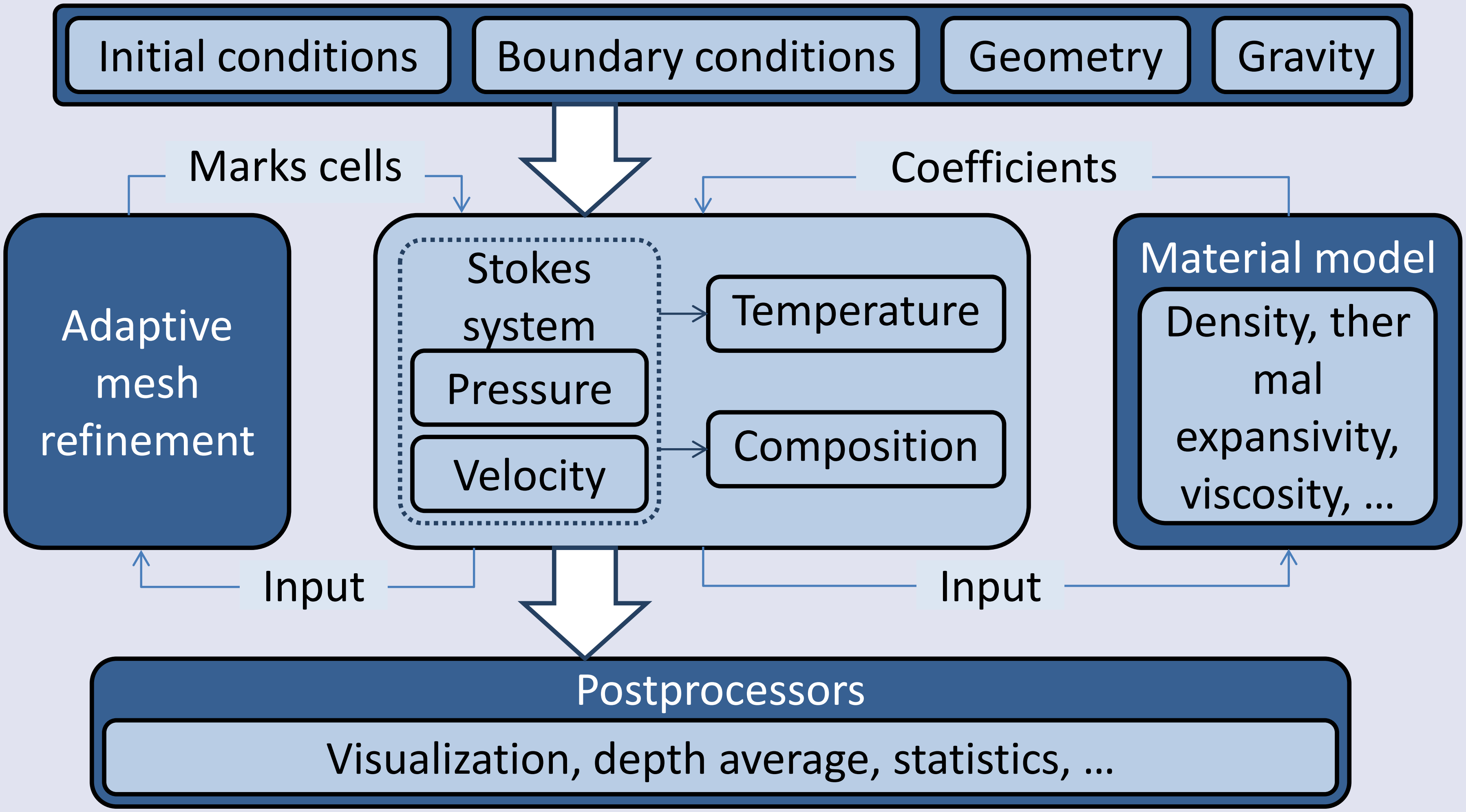
```
subsection Gravity model
   set Model name = vertical
   subsection Vertical
     set Magnitude = 9.8
   end
 end

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

Modularity



Model setup
Adaptive mesh refinement
Simulator
Material model
Postprocessors

Modularity

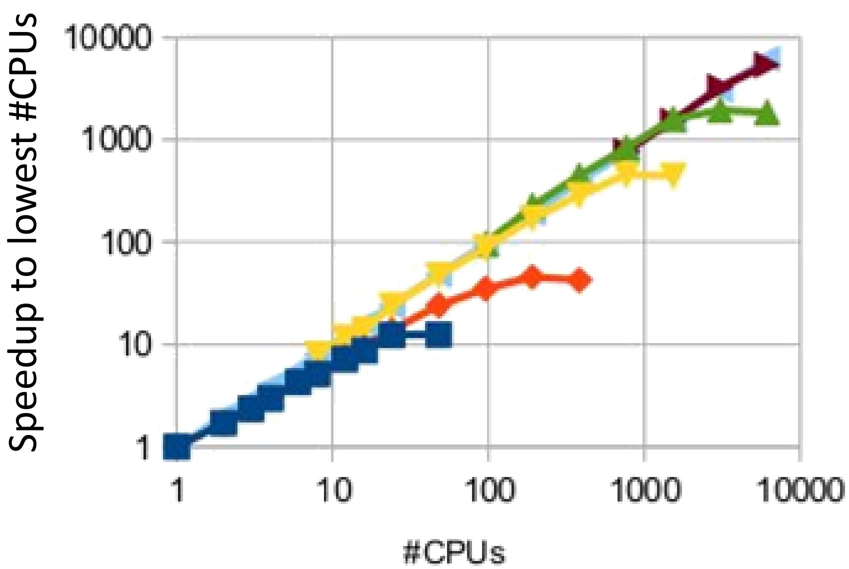


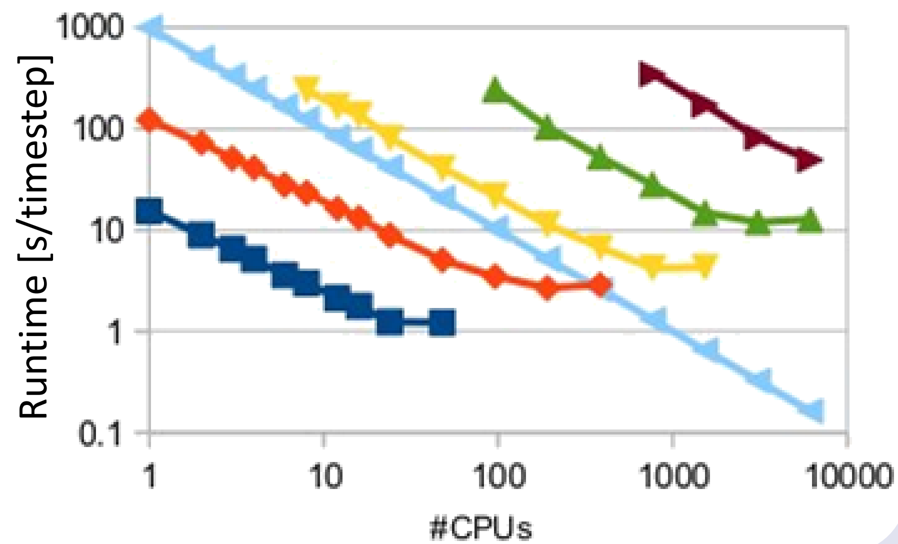
Initial conditions
Boundary conditions
Geometry
Gravity
Marks cells
Coefficients
Adaptive mesh refinement
Stokes system
Pressure
Velocity
Temperature
Composition
Material model
Density, ther mal expansivity, viscosity, …
Input
Input
Postprocessors
Visualization, depth average, statistics, …

Scaling

Speedup to maximal #DOFs/CPU

Strong Scaling





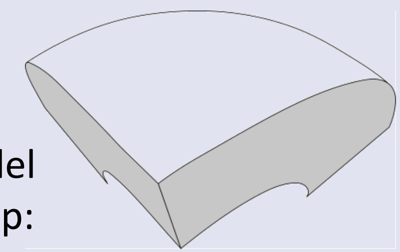
#DOFs

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

Resolution in km

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

Model Setup:



Scales almost linearly = excellent parallelization!

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

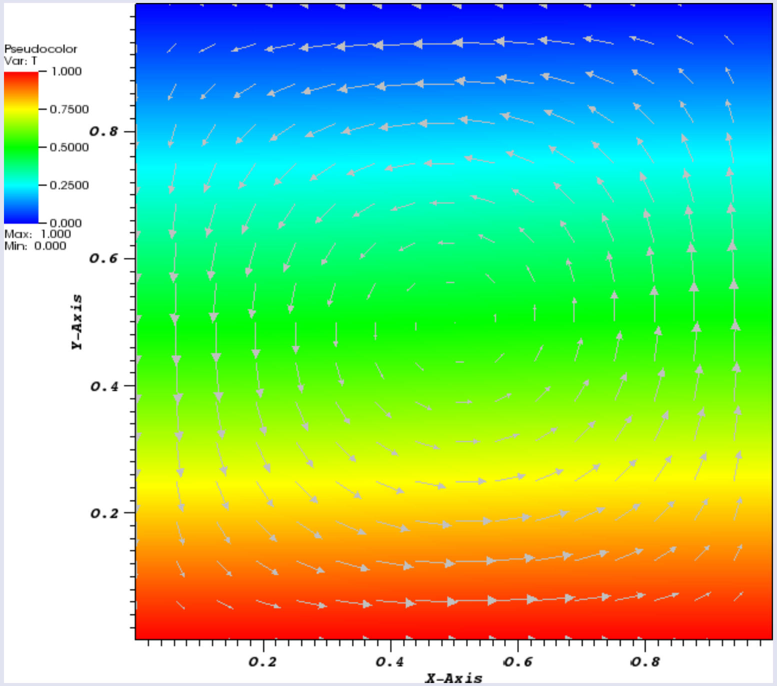
Exercise 1
Convection in a 2D Box

Nusselt-Rayleigh Relationship & Visualization with ParaView

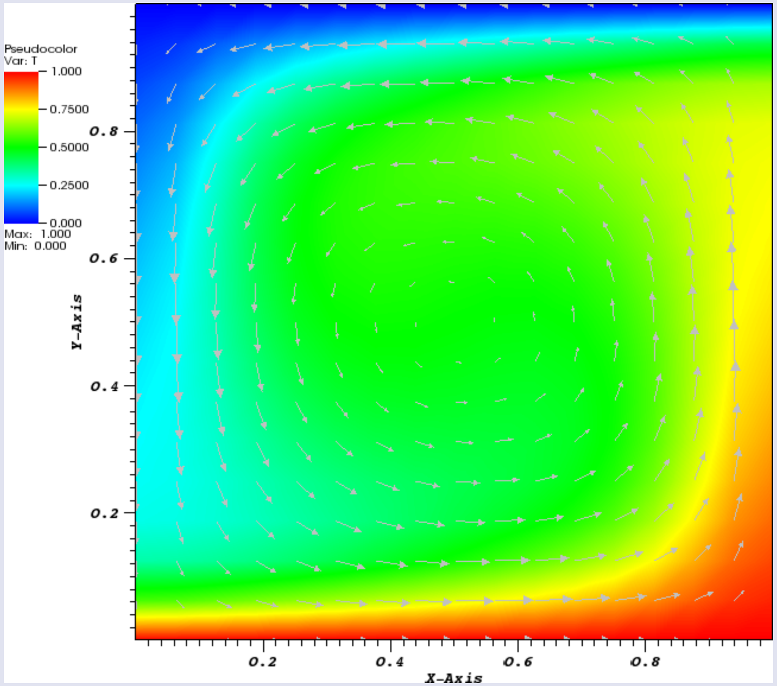
Nusselt-Rayleigh Relationship

Convection in a 2D Box

(free slip boundaries)



Initial temperature and velocity field



Final temperature and velocity field

Nusselt-Rayleigh Relationship

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

- In this tutorial, you control the Rayleigh number Ra with the viscosity η:

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

Ra = dimensionless parameter, indicates the presence and strength of convection in the mantle

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

$$= \frac{5.0993 \times 10^{28}}{Ra}$$

ρ_0 = reference density
g = gravity acceleration
α = thermal expansion coefficient
T = temperature
D = depth
κ = thermal diffusivity

Nusselt-Rayleigh Relationship

- Nusselt number Nu = the ratio of convective to conductive heat transfer,

  related to the surface heat flux

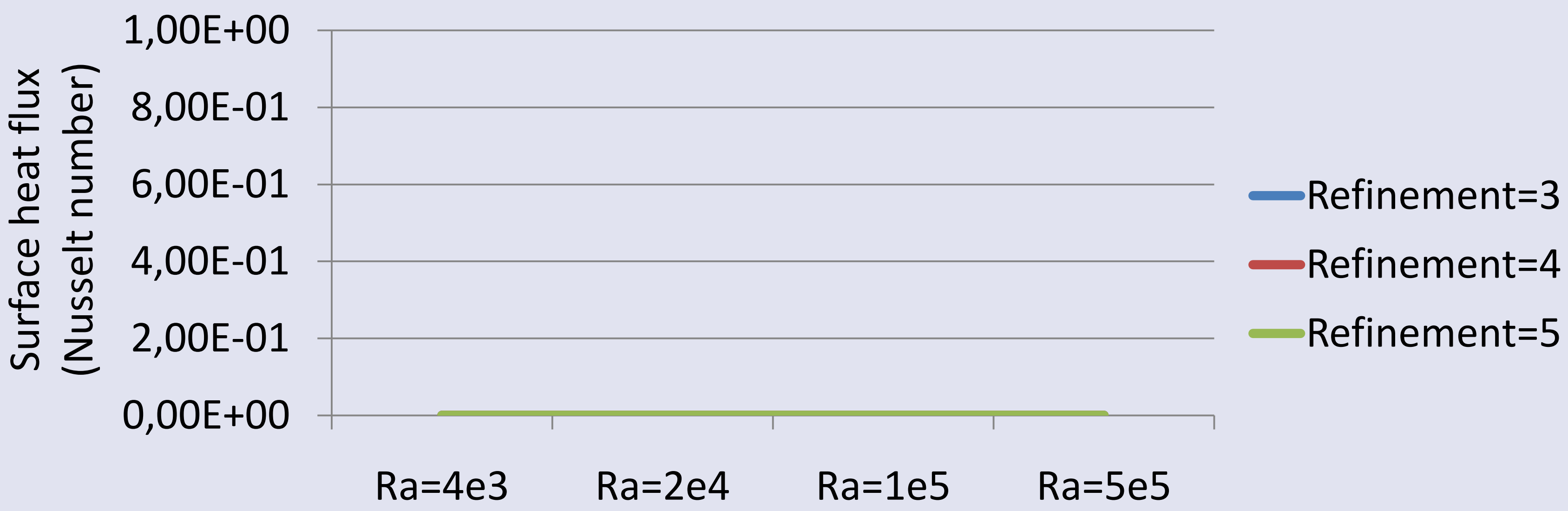
Questions

- 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

	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	(???)	(???)	(???)	(???)



Nusselt-Rayleigh Relationship

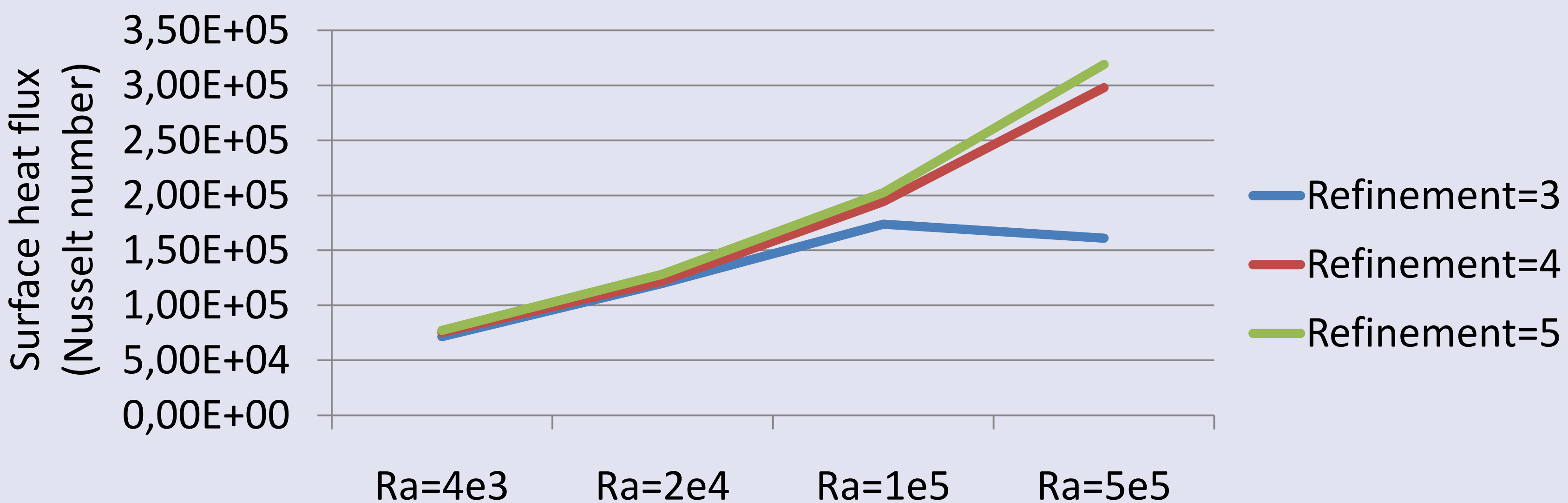
COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

1. Modify the refinement, end time, and Rayleigh number in tutorial.prm
2. Run ASPECT with the tutorial parameter file
   aspect tutorial.prm
3. Look at the log
   gedit output/log.txt
4. Look at the statistics output
   gedit output/statistics
5. Plot the results in gnuplot (time vs. heat flux)
   gnuplot
   plot "output/statistics" using 2:20 with lines;

Just a hint: To stop the calculations, press Ctrl + C

Nusselt-Rayleigh Relationship

	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	**7.14e4**	**1.20e5**	**1.74e5**	**1.61e5**
Refine = 4	**7.54e4**	**1.22e5**	**1.94e5**	**2.98e5**
Refine = 5	**7.72e4**	**1.28e5**	**2.02e5**	**3.19e5**



Nusselt-Rayleigh Relationship

- If the Rayleigh number goes up, how does the Nusselt number change?

  if Ra goes up → Nu goes up

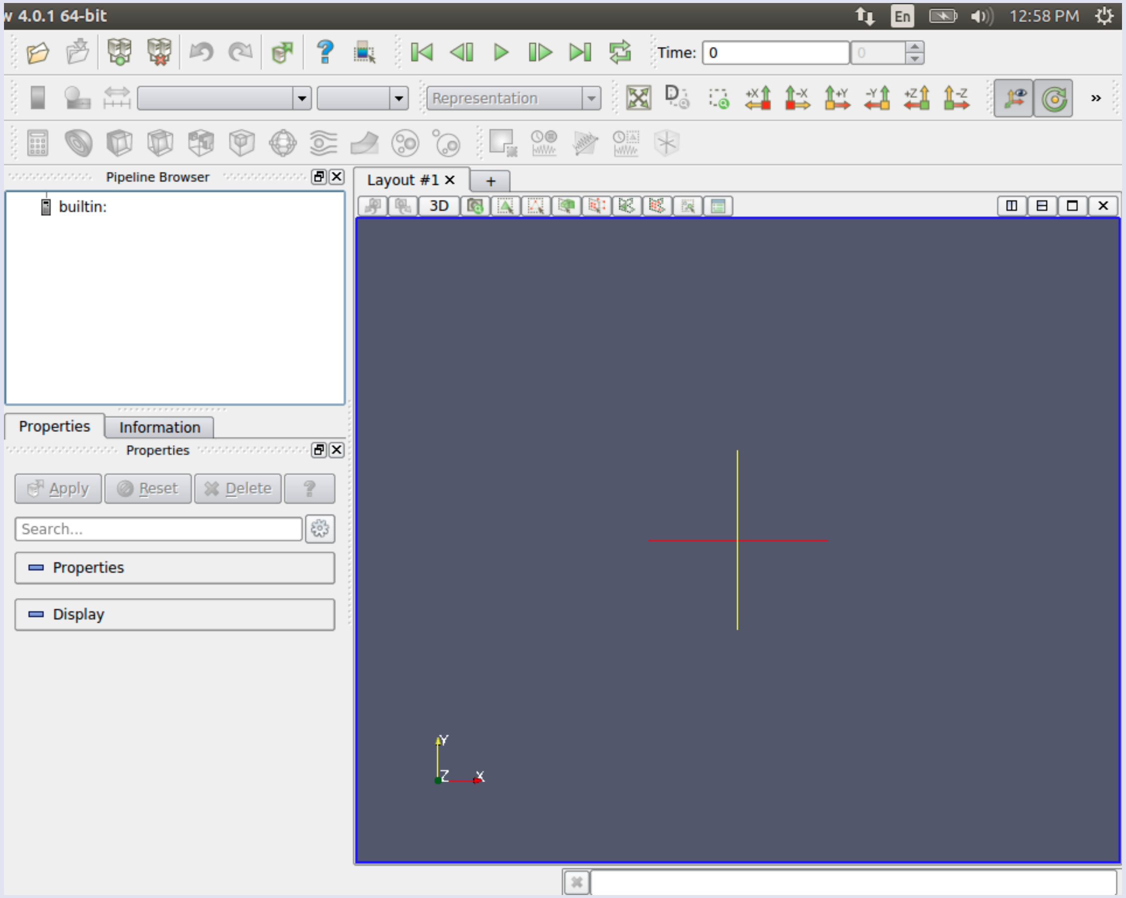
- How does the mesh resolution affect the accuracy of these results?

  if mesh refinement is too low, the result for high Ra is no longer accurate!

Visualization with ParaView

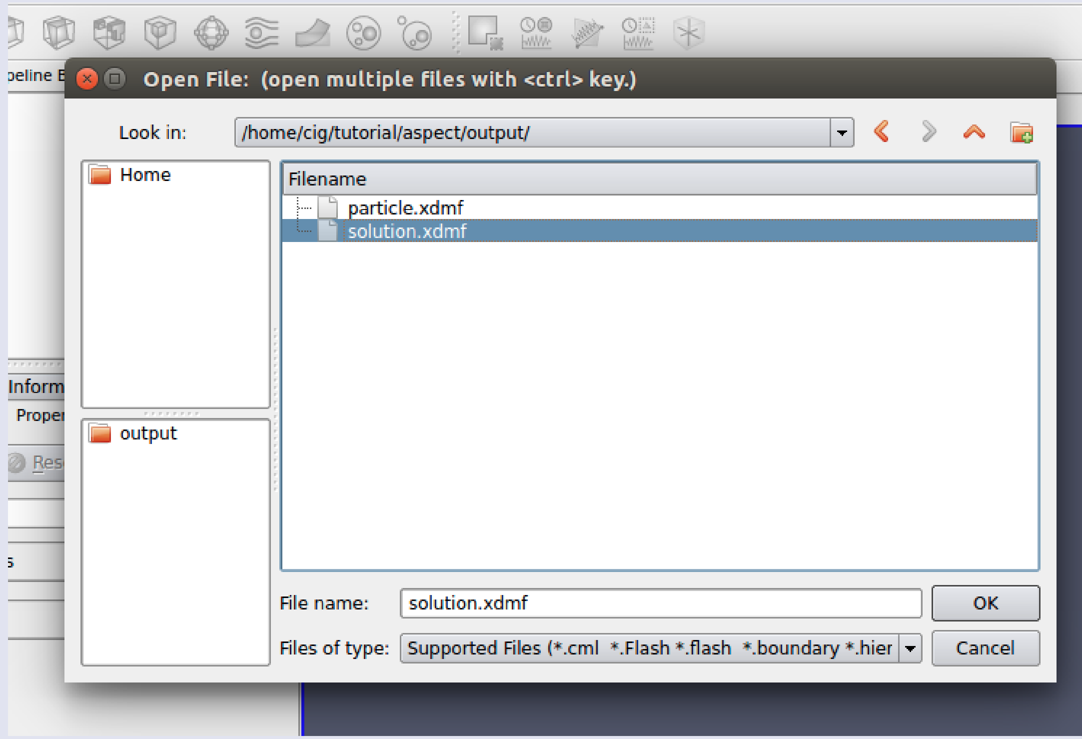
CIG COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

ParaView = program for visualization of large data sets



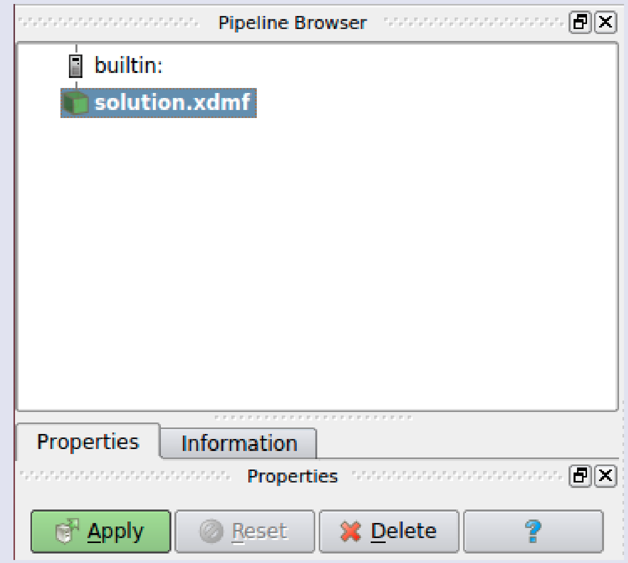
Visualization with ParaView

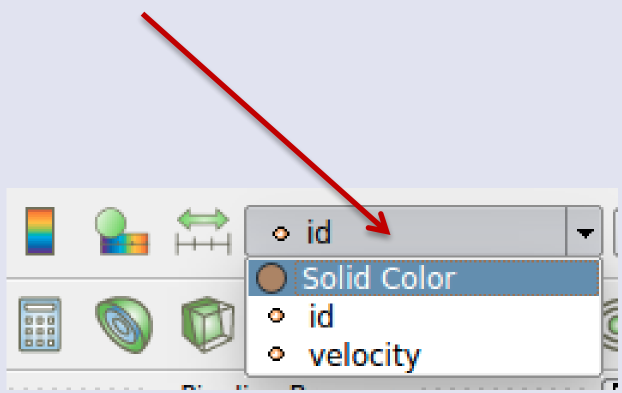
- Aspect creates the file solution.pvd
- choose "Open" from the File menu
- The file is in ASPECT_TUTORIAL/models/output/

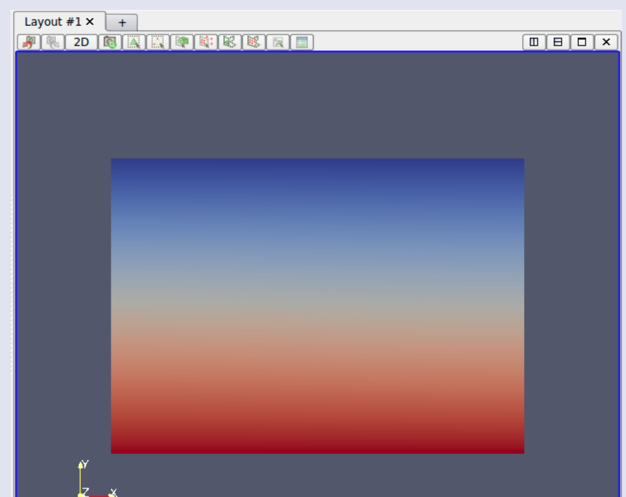


Visualization with ParaView

- the file contains the variables temperature (T), pressure (p), and velocity
- click “Apply” + Select “T” in the toolbar to show the temperature field



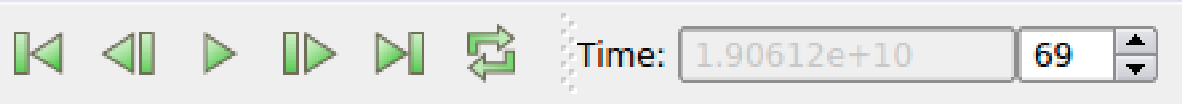




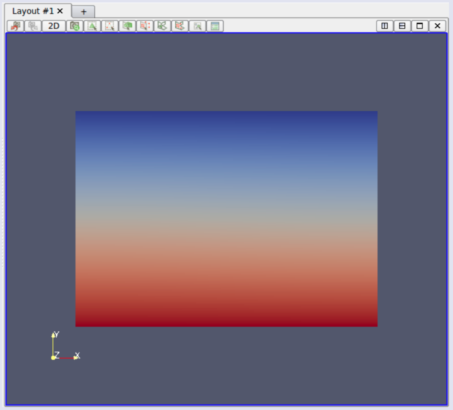
Visualization with ParaView

- change the time in the top toolbar + click "Play"

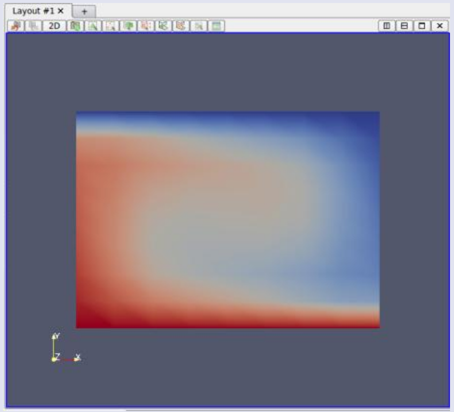
Previous Frame
Next Frame
Loop



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



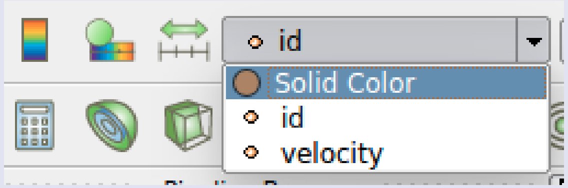
Frame 0



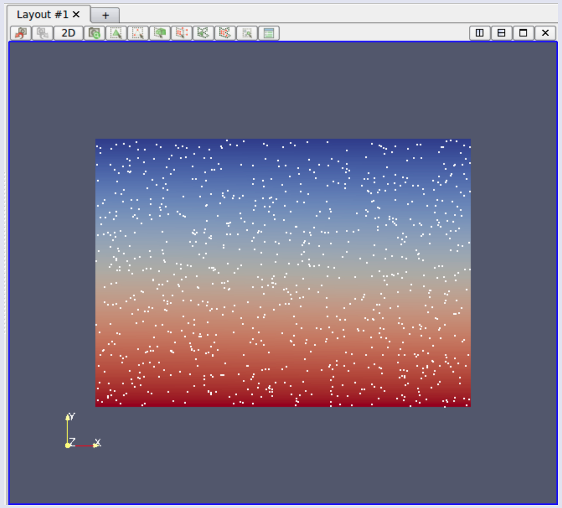
Frame 231

Visualization with ParaView

- Open the file particle.pvd and click “Apply” to see the tracer particles
- Click “play” to see how material is flowing with the tracer particles



Change the coloring scheme to “Solid Color”

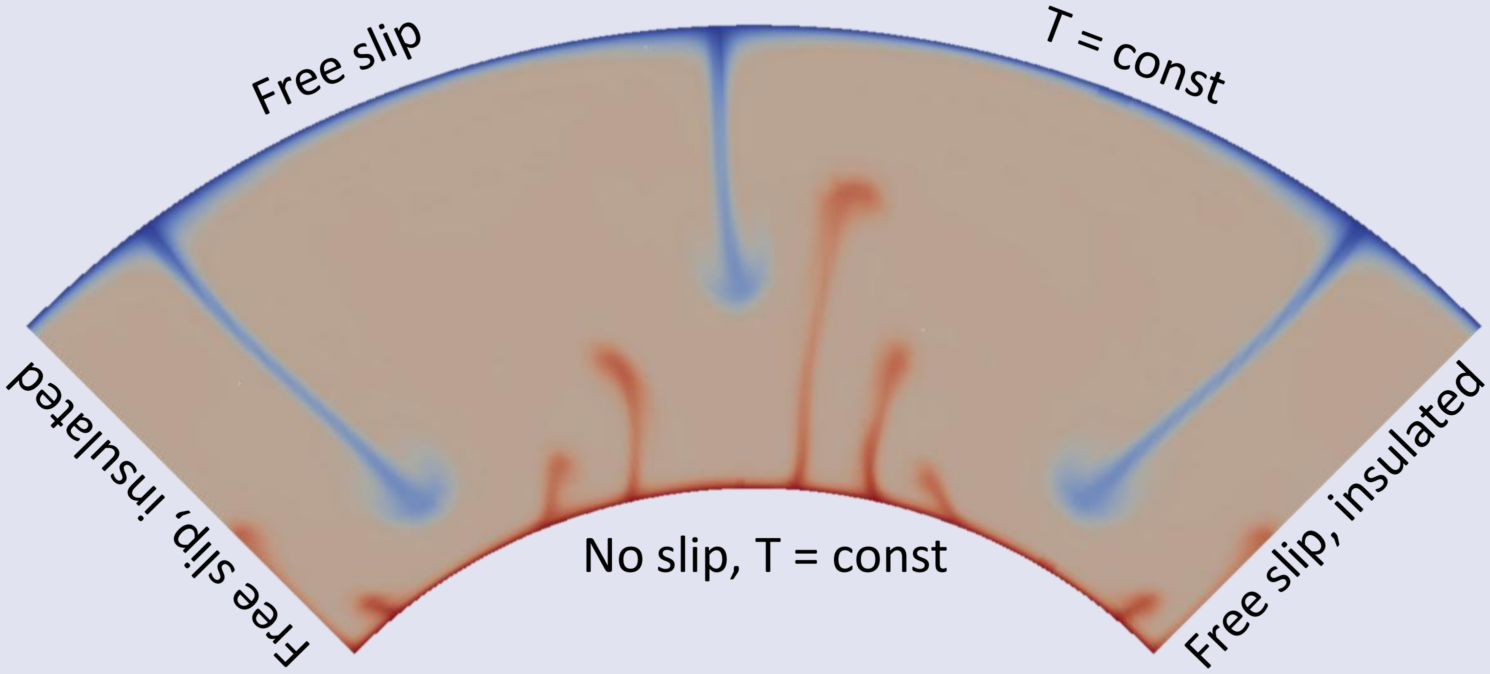


Temperature field with tracer particles

Exercise 2
Convection in a 2D spherical shell

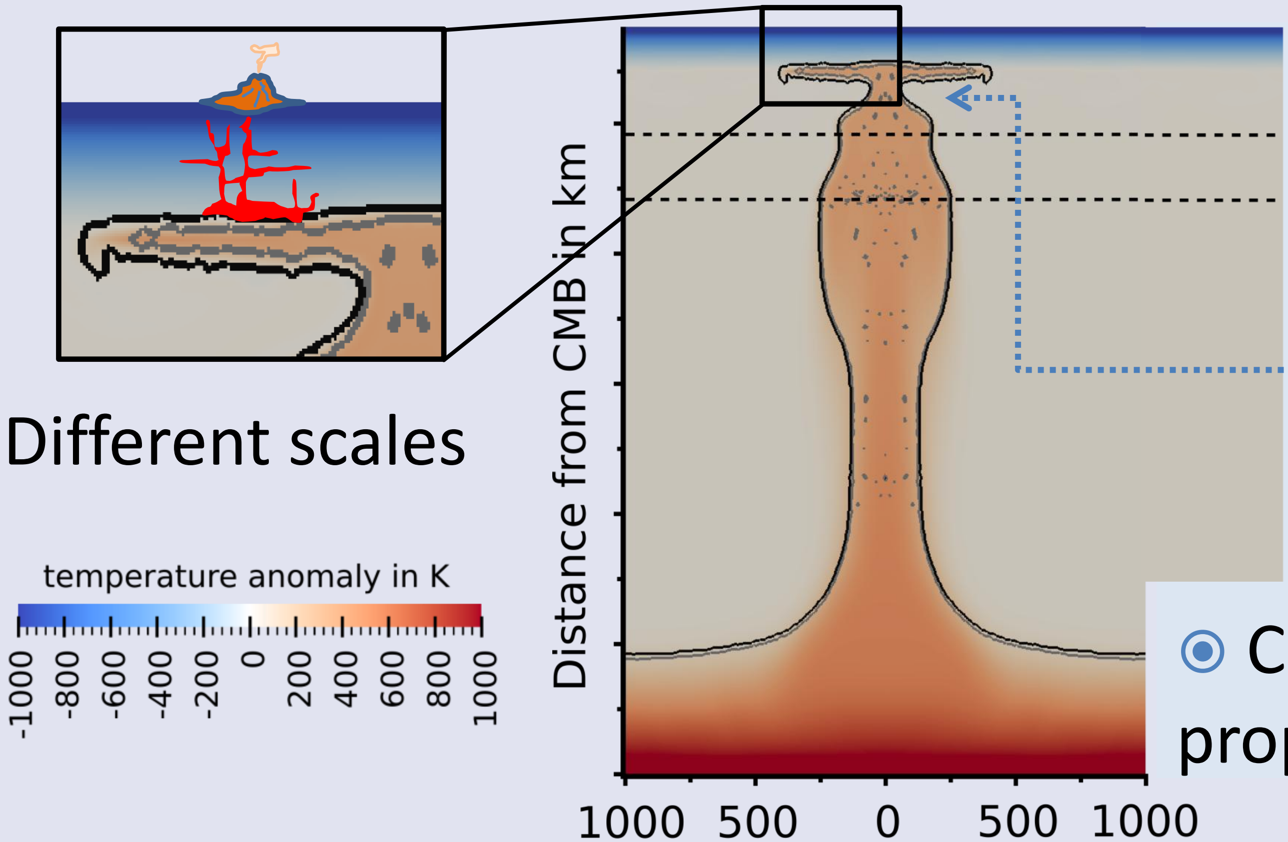
Adaptive mesh refinement & Spherical shell geometry & Visualization

Setup: Convection in a Shell



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

Numerical Challenges



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

Questions:

- How does the flow field change with varying the resolution?
- How does the runtime change with the adaptive refinement compared to global refinement?

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

```
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

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

```
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

Boundary conditions

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

```
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

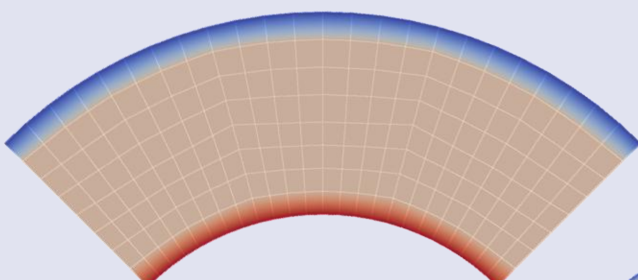
Exactly the same as:

```
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
```

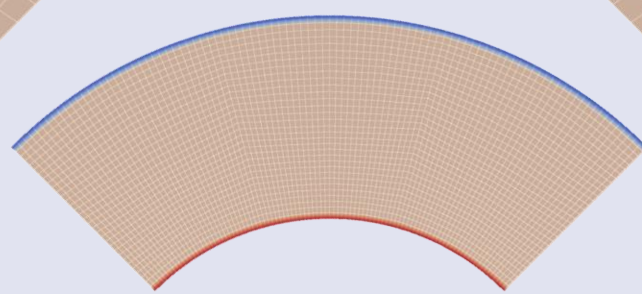
Mesh refinement

This is what needs to be changed:
Group 1: 3, Group 2: 4, Group 3: 5

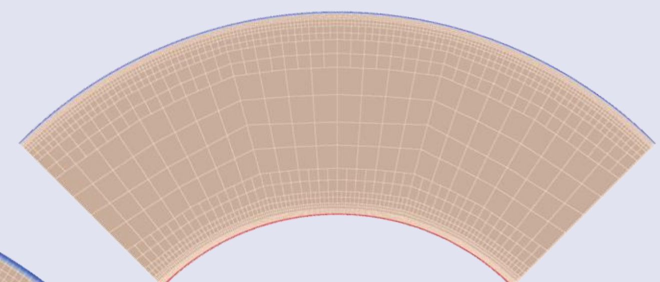
```
subsection Mesh refinement
  set Initial global refinement                = 5
  set Initial adaptive refinement              = 0
  set Strategy                                 = temperature
  set Time steps between mesh refinement = 0
  set Coarsening fraction                      = 0.05
  set Refinement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



Global refinement = 3



Global refinement = 5



Global refinement = 4
Adaptive refinement = 2

Tasks

1. Modify the spherical_shell.prm file to use your assigned refinement number
   gedit spherical_shell.prm
2. Run the simulation
   aspect spherical_shell.prm or in parallel
   mpirun –np 2 aspect spherical_shell.prm
3. Visualize the results with Paraview
   ASPECT_TUTORIAL/models/spherical-shell/ouput.pvd

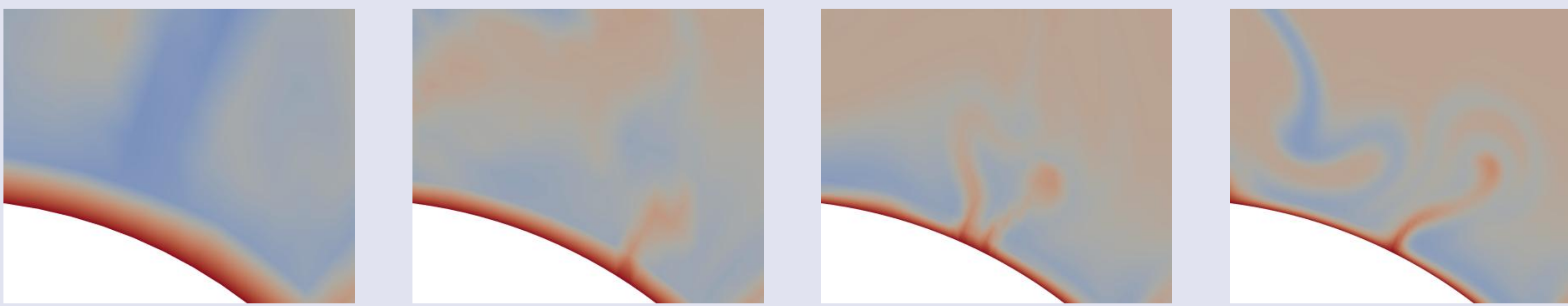
Just a hint: To stop the calculations, press Ctrl + C

Results

How does the flow field change with varying the resolution?

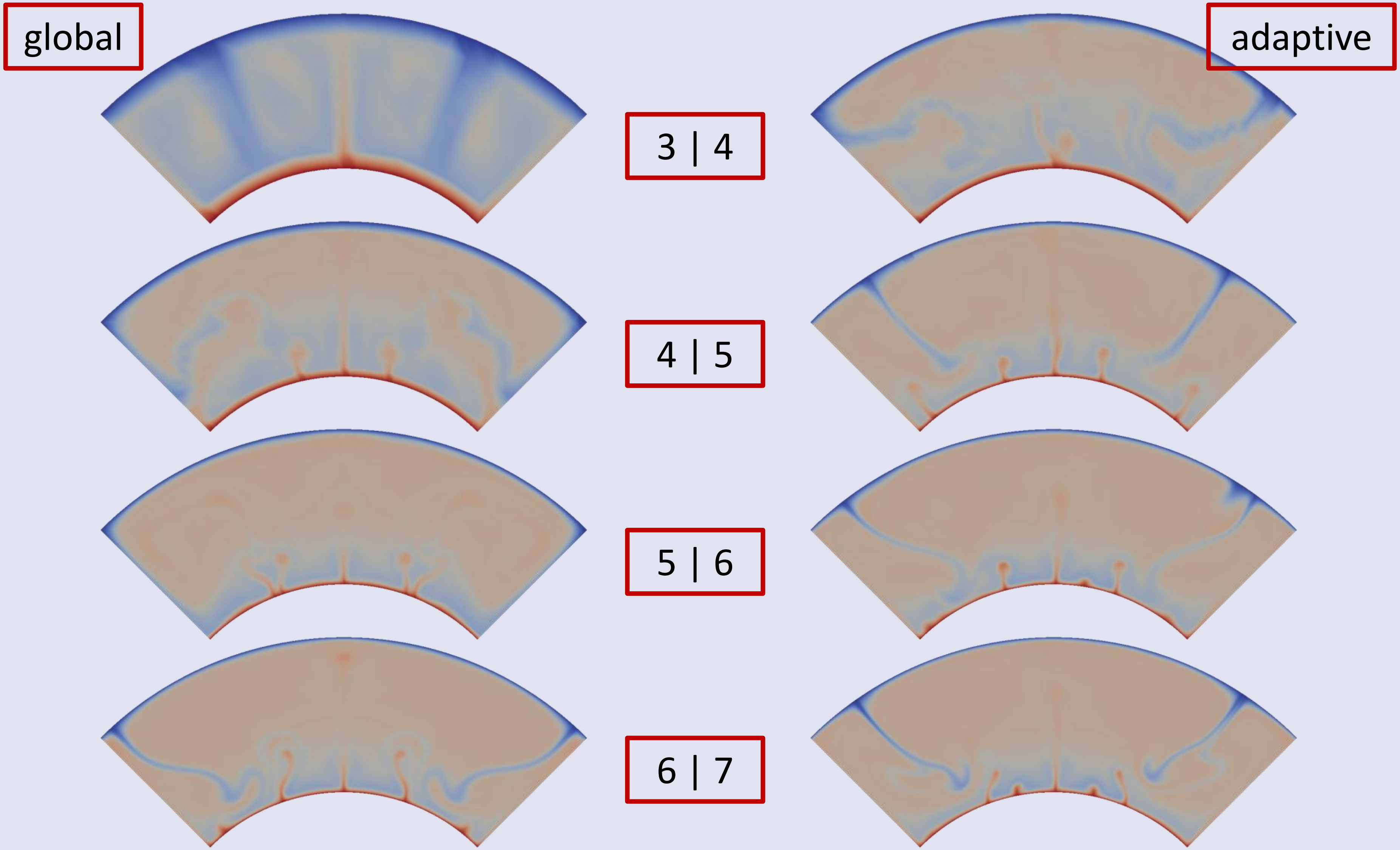
Time snapshots of models with different resolution

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



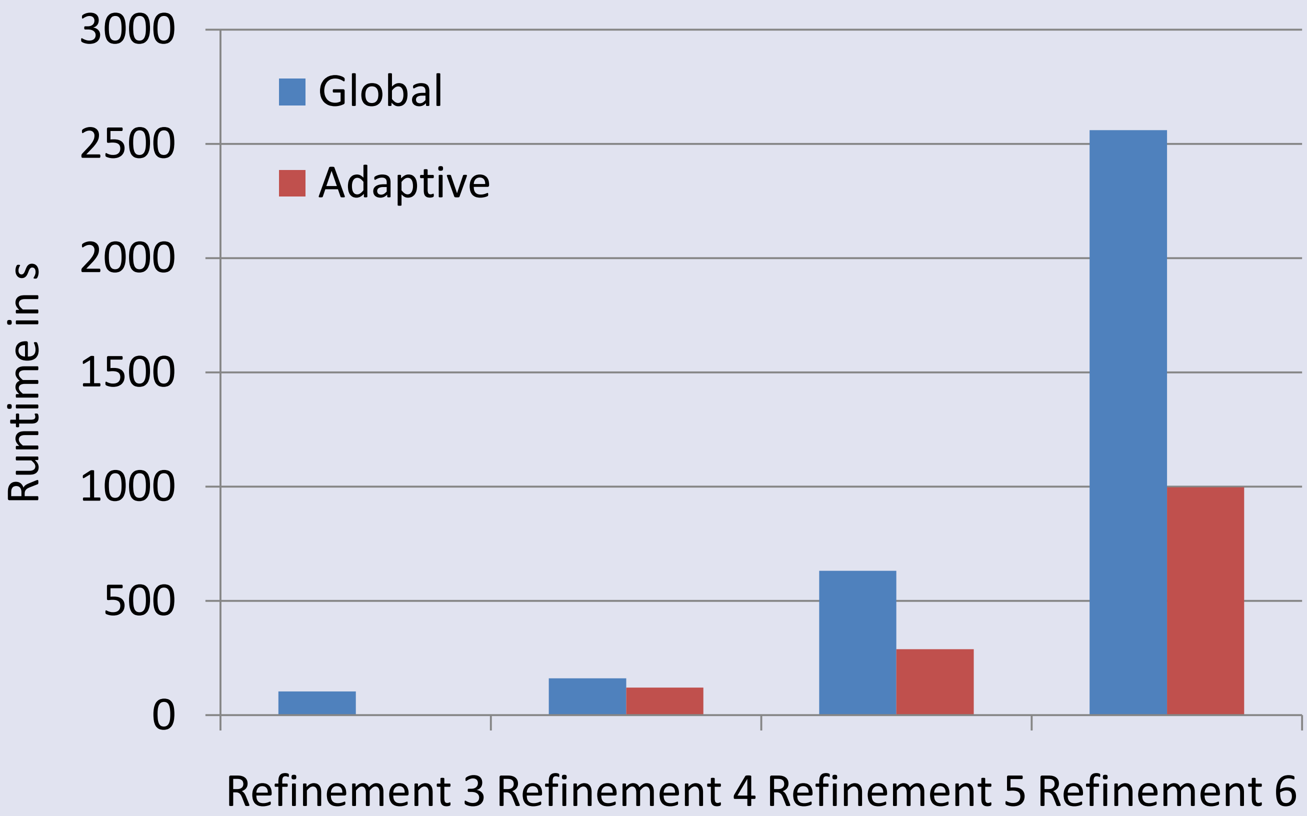
Results

How does the flow field change with varying the resolution?



Results

How does the runtime change with the adaptive refinement compared to global refinement?



[Movie: Earth Dynamic]

[Movie: Thermochemical convection of a mantle plume]