COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

First Steps
Running and Compiling ASPECT

GeoMod2014

Credits

Website and manual:

aspect.dealii.org

Developers & contributors:

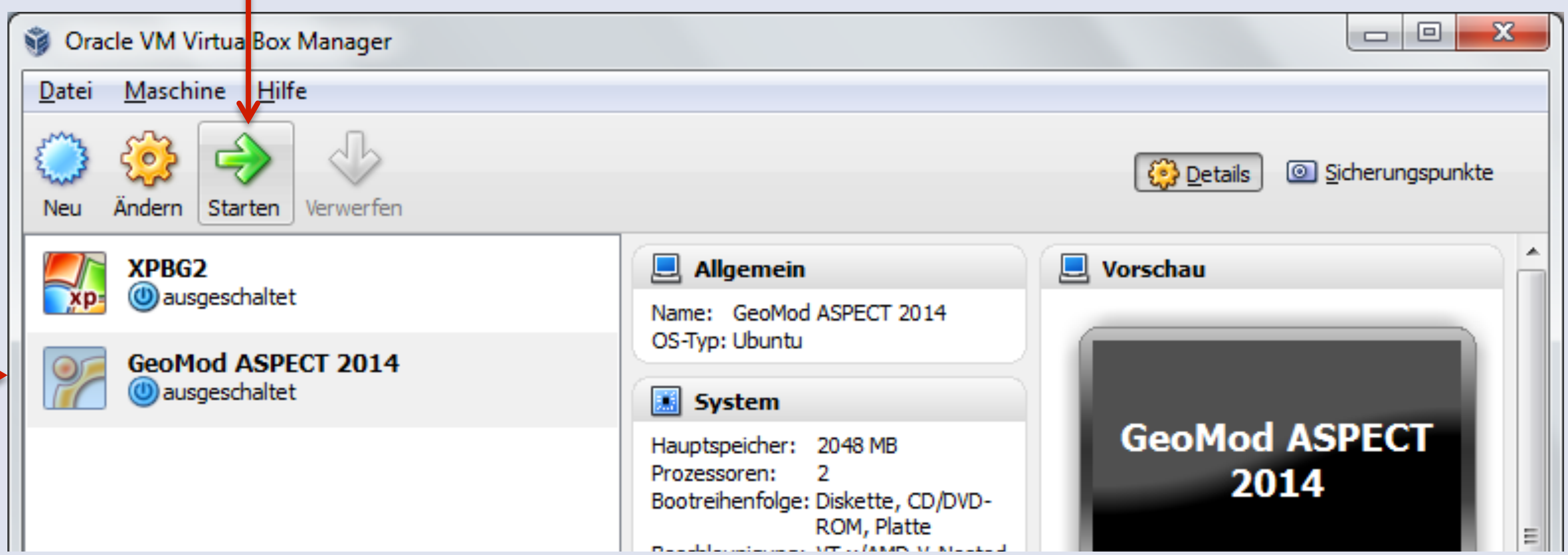
Wolfgang Bangerth,
Timo Heister and many more

Publication:

Kronbichler et al. 2012 GJI

Aspect in the virtual machine

- Start VirtualBox on your computer
- Start the **GeoMod ASPECT 2014** virtual machine



Compiling ASPECT

1. Start the terminal

```
cd ASPECT_TUTORIAL/aspect/release
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)
```

```
make –j2
```

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

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- We will begin by running ASPECT in the Terminal

1. Change to the appropriate directory

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

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 > progress.txt
```

3. Open progress.txt and check the Rayleigh number

```
gedit progress.txt
```

Debug or Optimized mode?

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- 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

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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

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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

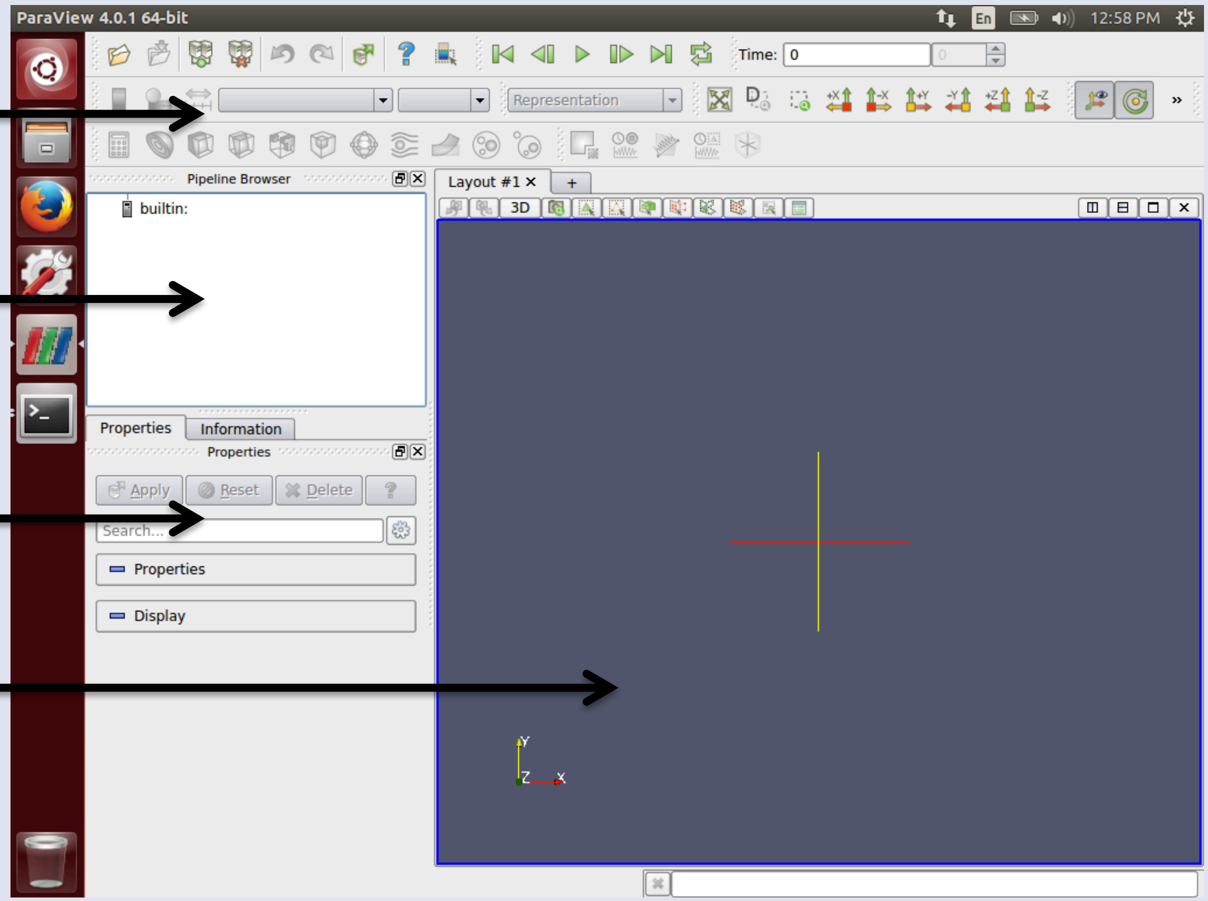
Visualization with ParaView

Toolbars

Pipeline Browser

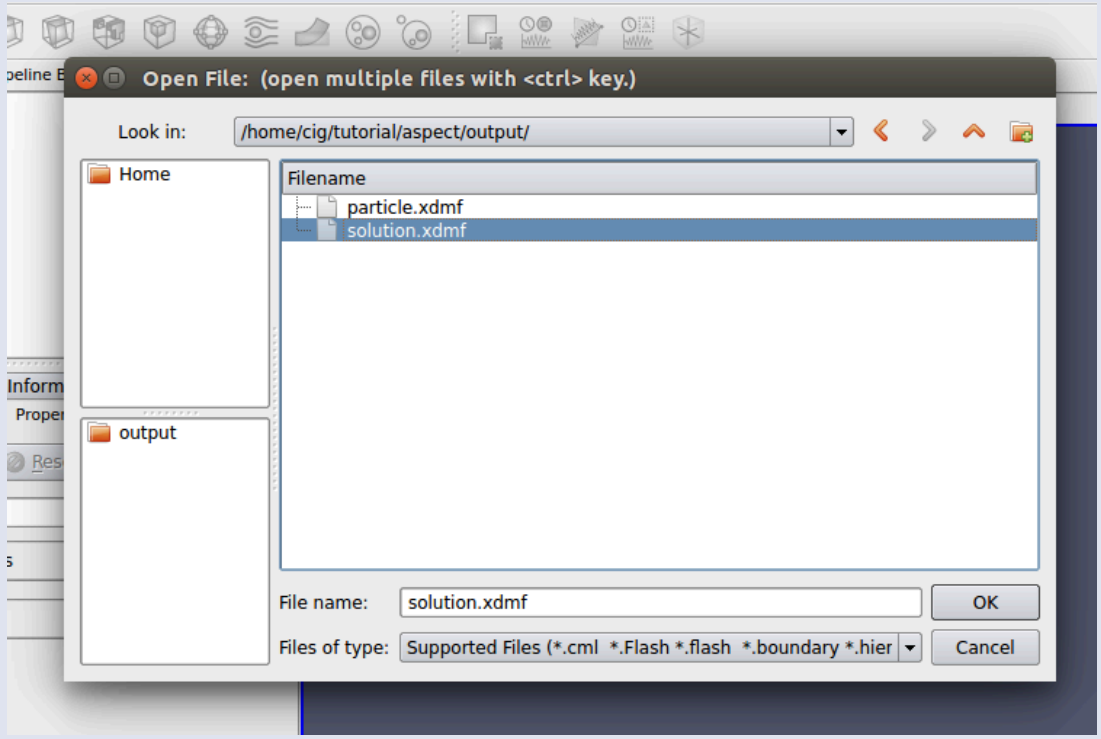
Object Inspector

2D/3D View



Visualization with ParaView

- Start by opening solution.pvd 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/ASPECT_TUTORIAL/models/output/



Visualization with ParaView

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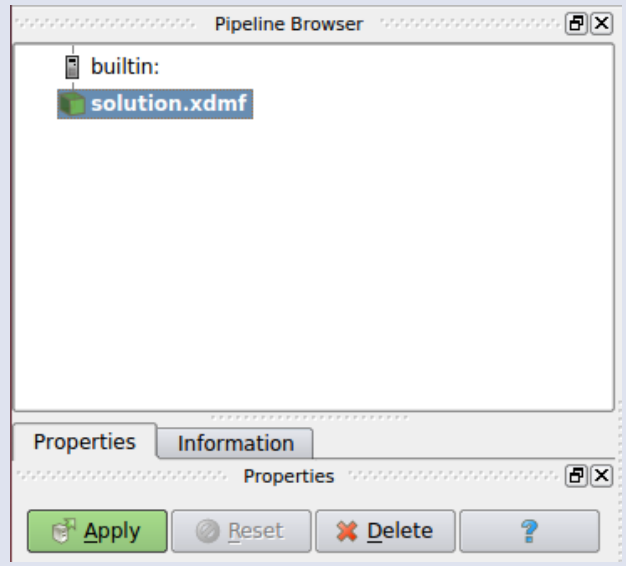
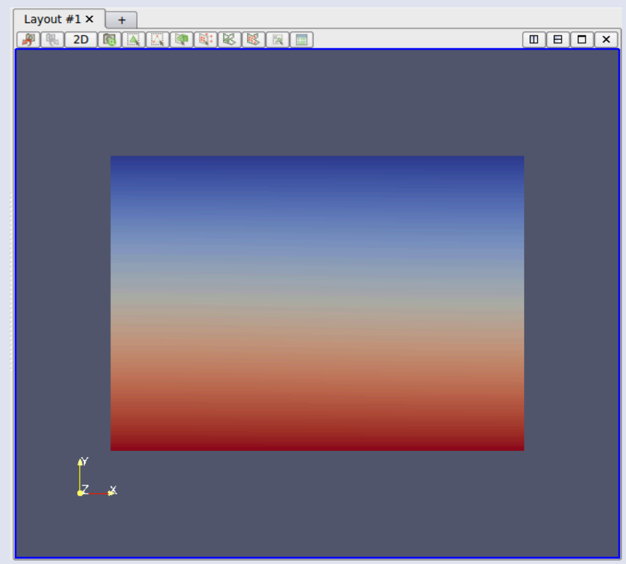
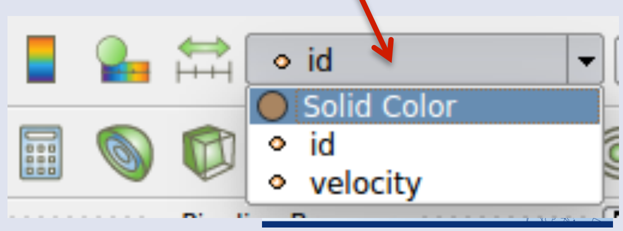
- The file will appear in the pipeline browser
  – Make sure this is solution.pvd
- The list of properties (variables) appears in the object inspector
  – The file contains temperature (T), pressure (p), and velocity
- Click "Apply" to show the field in the view area
  – By default, no field is shown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







Visualization with ParaView

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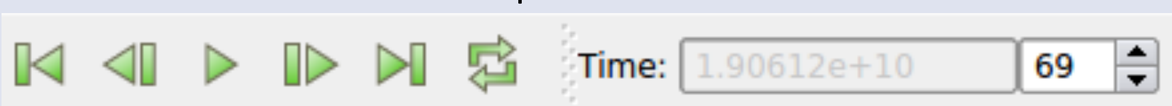
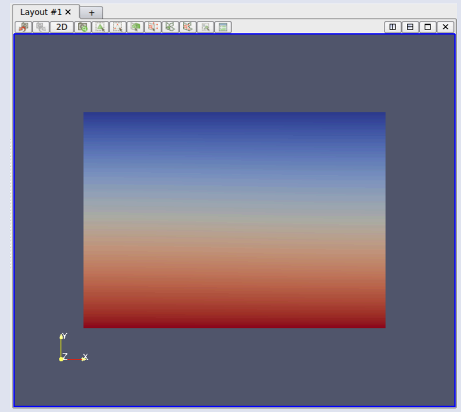
- The top toolbar has buttons to change the time, shown below
  - Click the play button and watch how the temperature field changes
  - Near the end, is the temperature field static? Is the velocity field static? Is material moving?

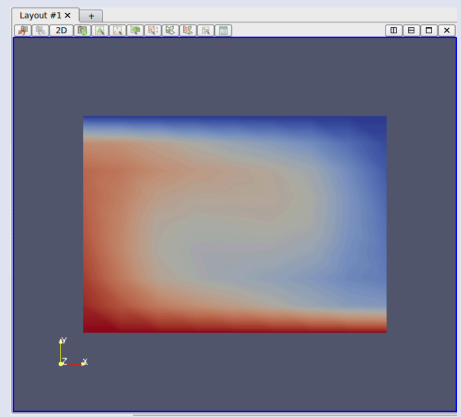
Previous Frame | Next Frame | Loop



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



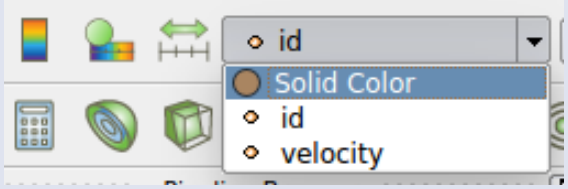
Frame 0



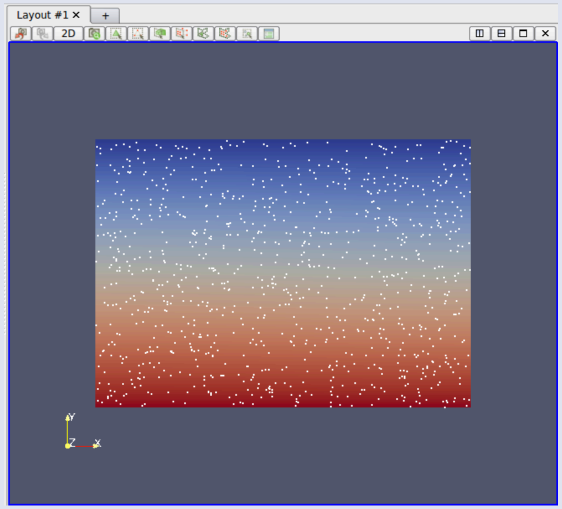
Frame 231

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 modelling software

Juliane Dannberg

GeoMod2014

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".

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

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

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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

Equations

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

Momentum equation

Divergence of stress tensor

Pressure gradient

Gravity force

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

(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	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	$\mathrm{Pa} \cdot \mathrm{s}$

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	$\frac{W}{m \cdot K}$
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Equations

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

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)

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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

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

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

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

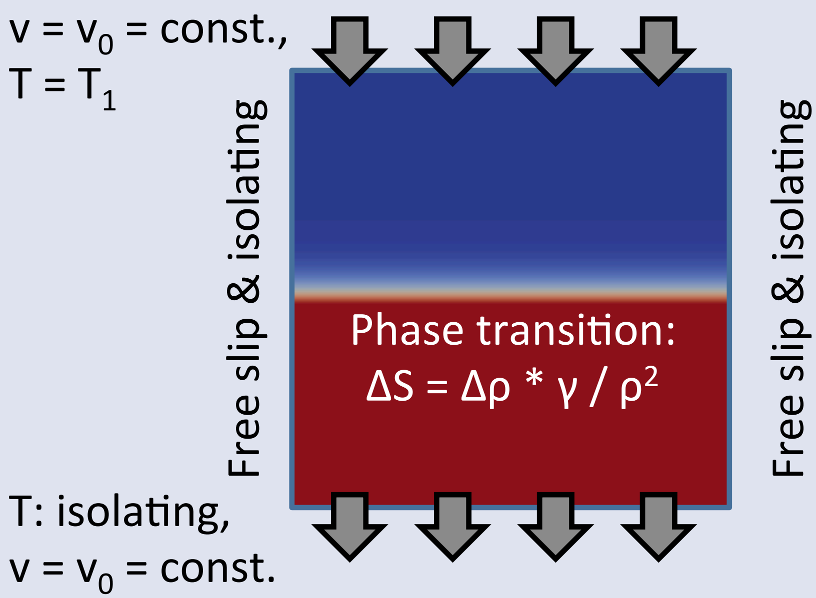
Advection of compositional fields

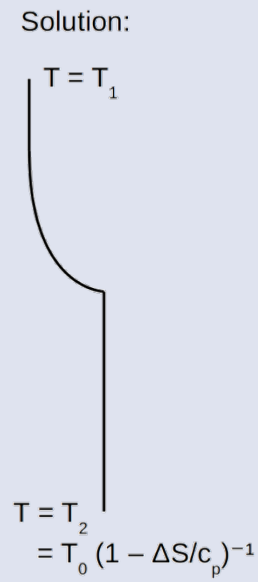
Field method (instead of tracer method)

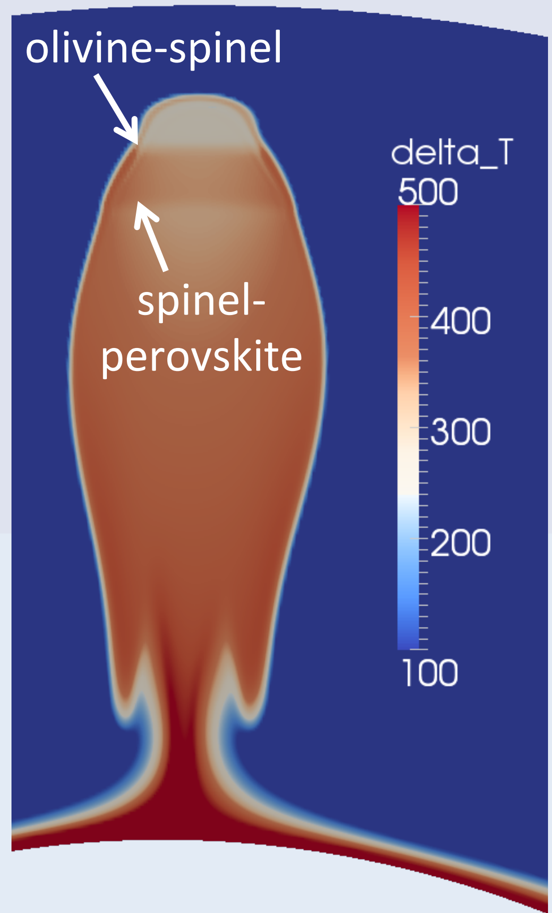
Equations

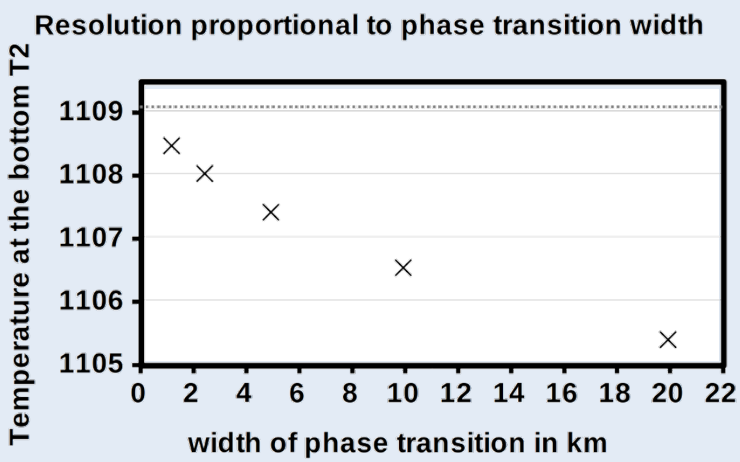
- Compressibility
- 2- or 3-dimensional domain Ω, different geometries
- Total pressure
- Radiogenic heating
- Adiabatic heating, shear heating & latent heat
- Advection of any number of compositional fields

Latent heat release









Numerical methods

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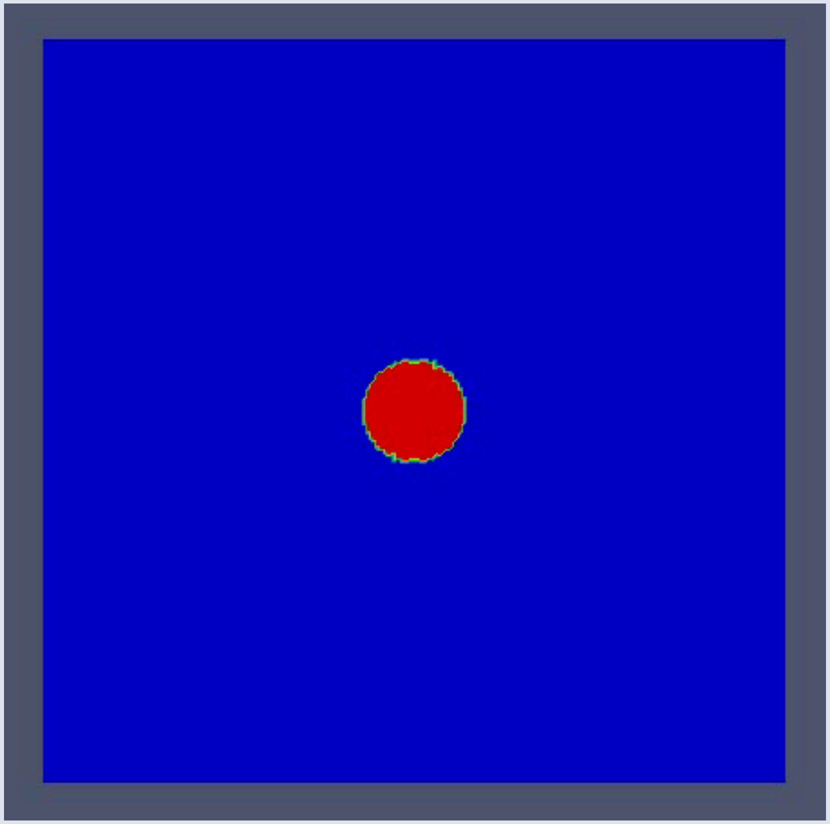
- Mesh adaptation
- Accurate discretizations (choice of finite element for velocity and pressure + nonlinear artificial diffusion for temperature stabilization)
- Efficient linear solvers (preconditioner + algebraic multigrid)
- Parallelization of all of the steps above
- Modularity of the code

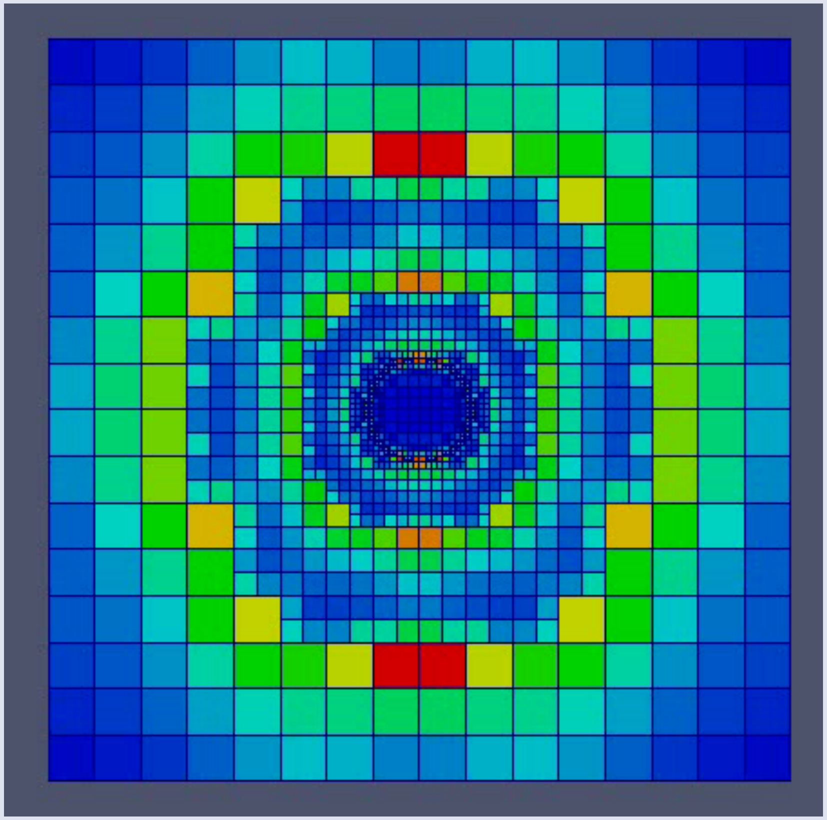
Mesh adaptation

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

- Example: Composition as refinement strategy



Compositional field



Mesh cells, colors indicate the estimated error

Mesh adaptation

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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***

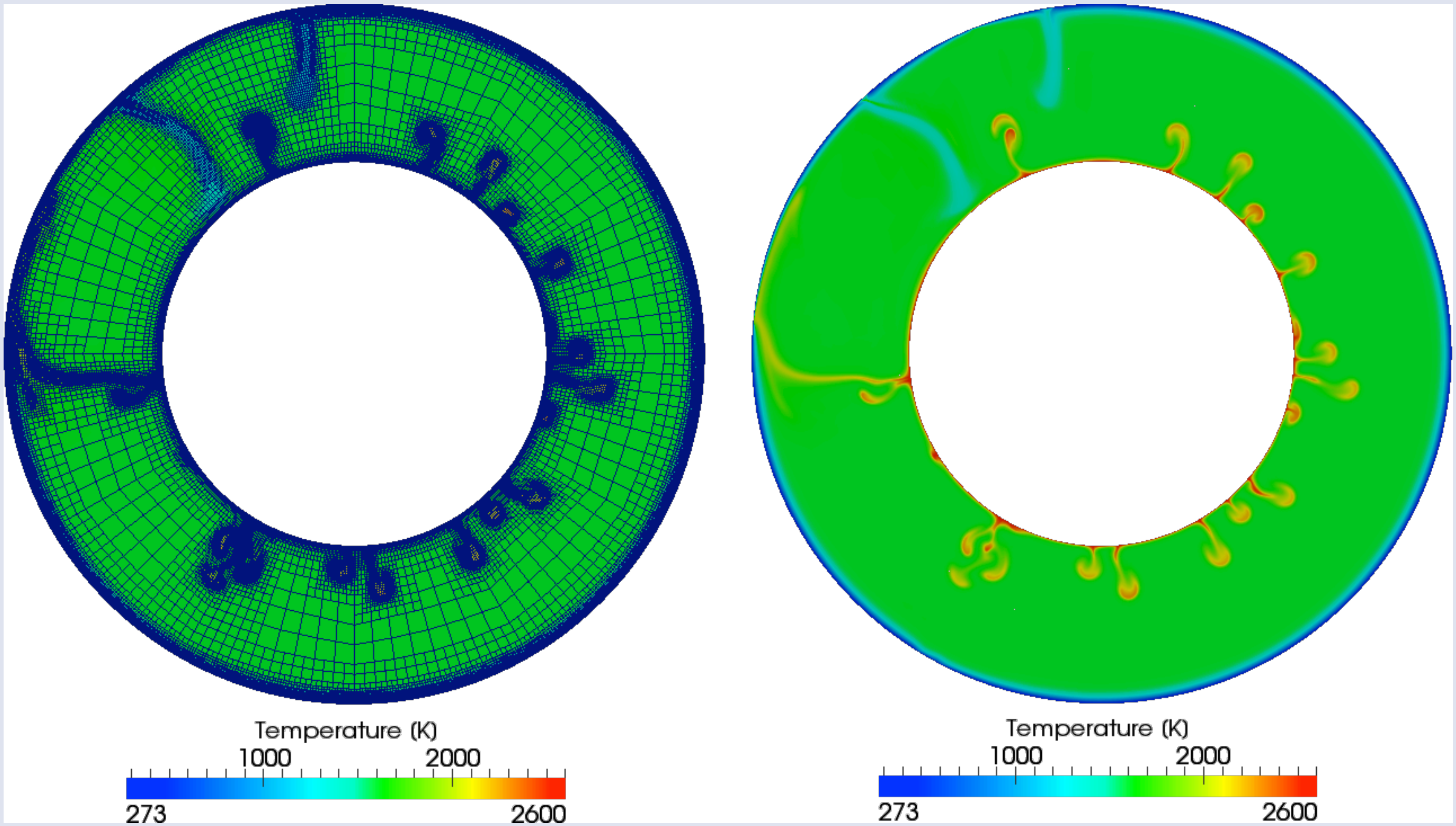
Look for the smallest subset M

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

(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



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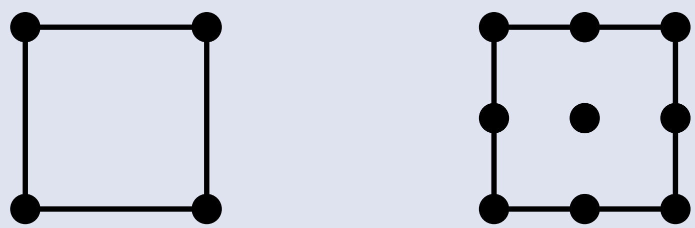
Discretization

- 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

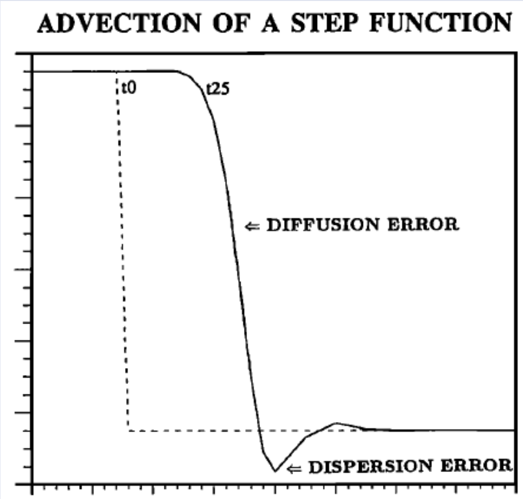


Velocity, temperature, composition

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



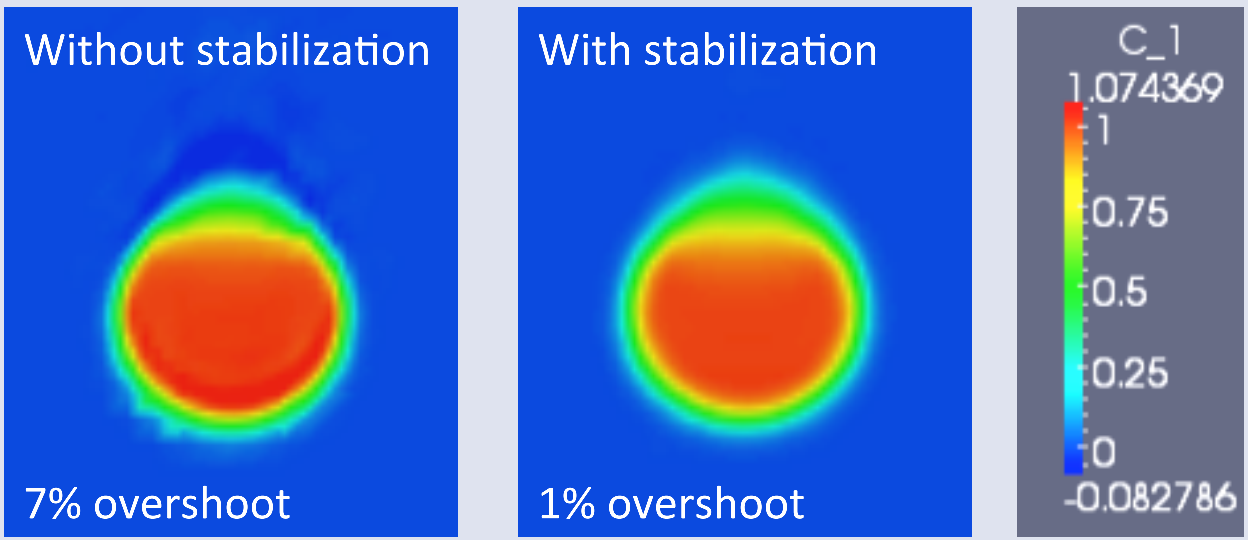
(Lenardic, Kaula, 1993)

Discretization

- Modified temperature/composition equation:

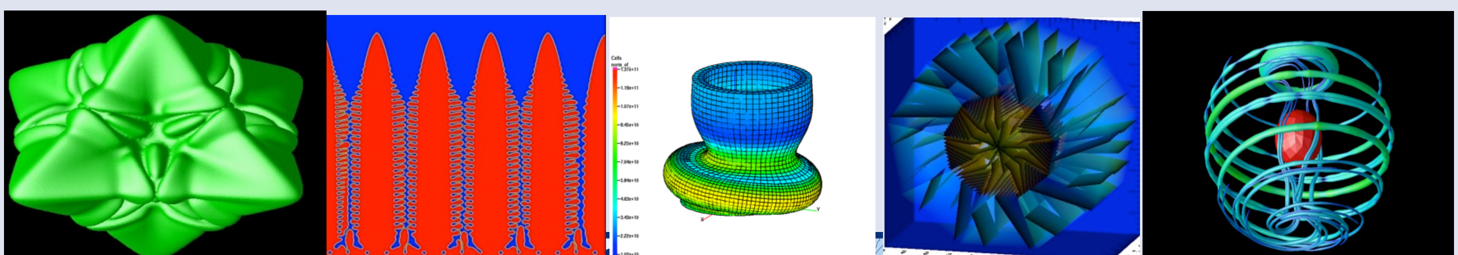
$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T - \nabla \cdot (\kappa + \nu_h(T))\nabla T = \gamma$$

- Result:



Aspect spatial discretization

- 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

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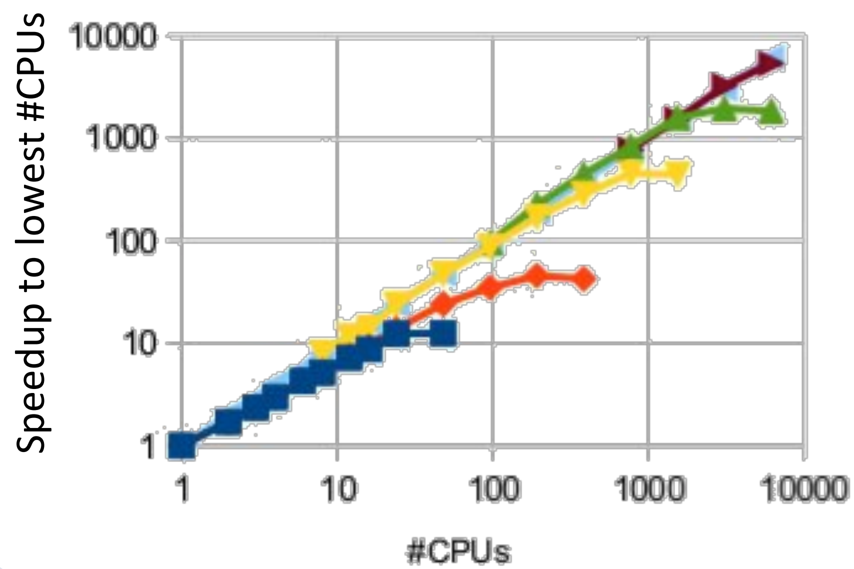
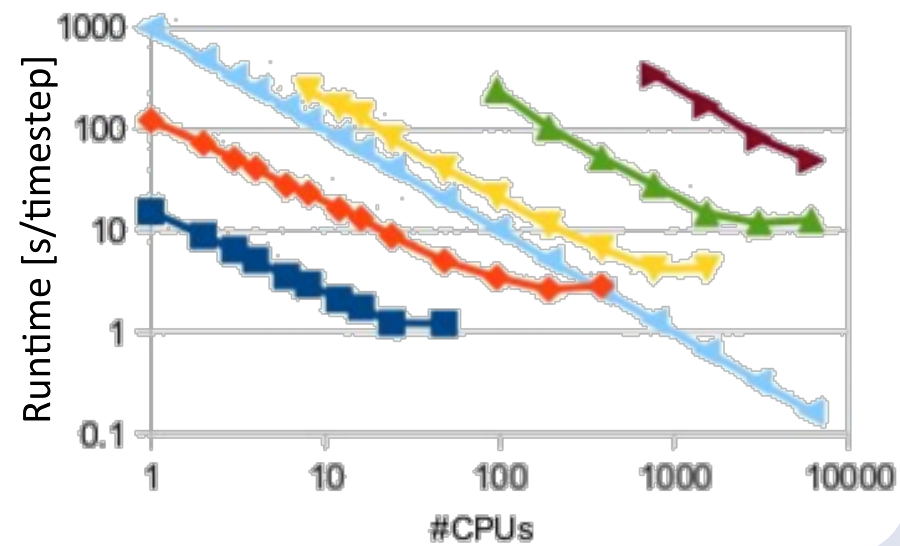
Speedup to maximal #DOFs/CPU



#DOFs

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

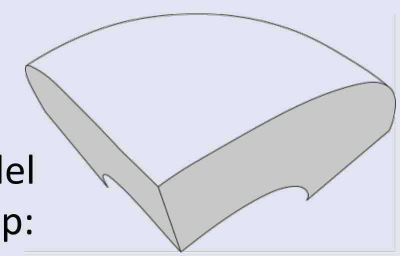
Strong Scaling



Resolution in km

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

Model Setup:



Work with R. Gassmoeller

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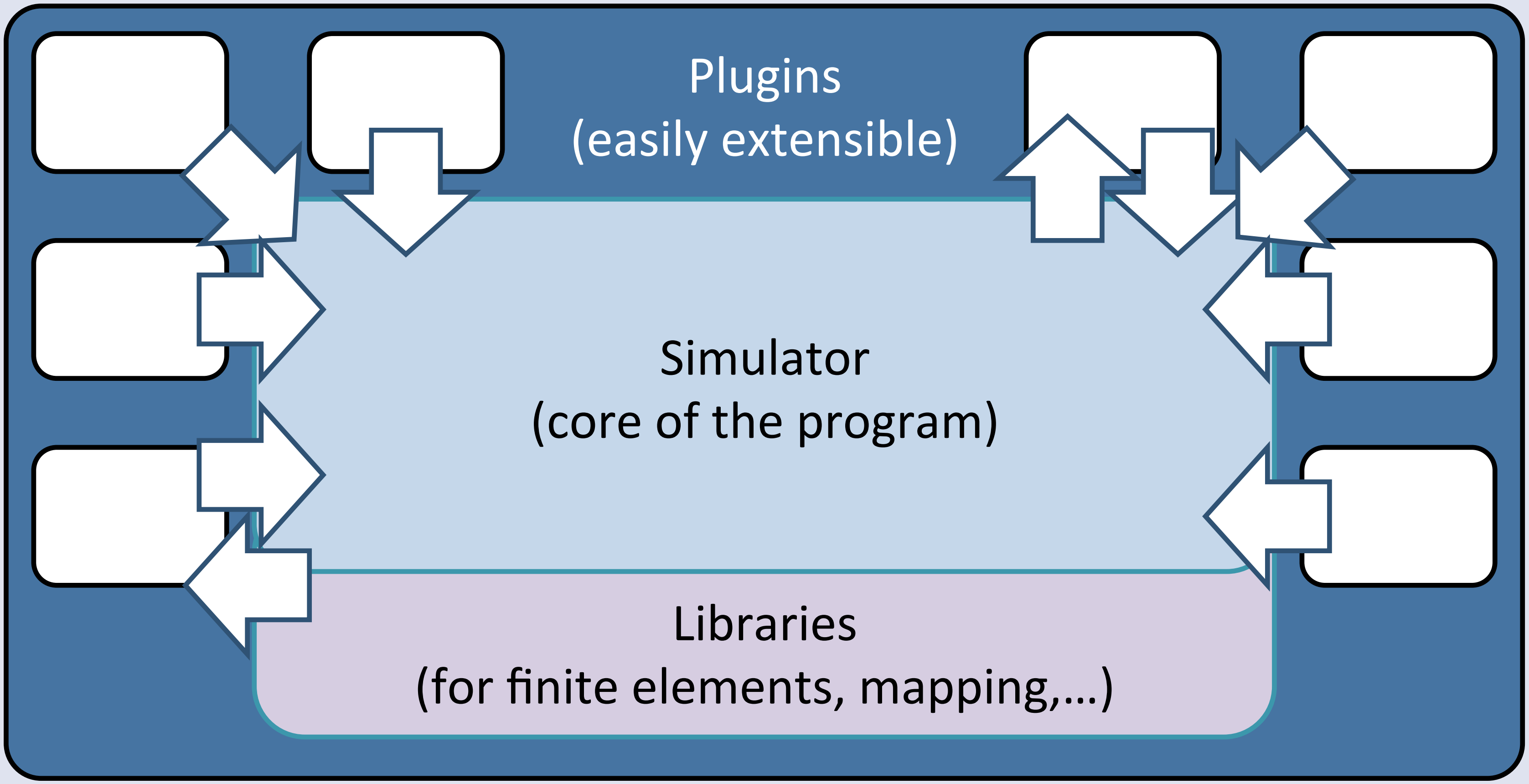
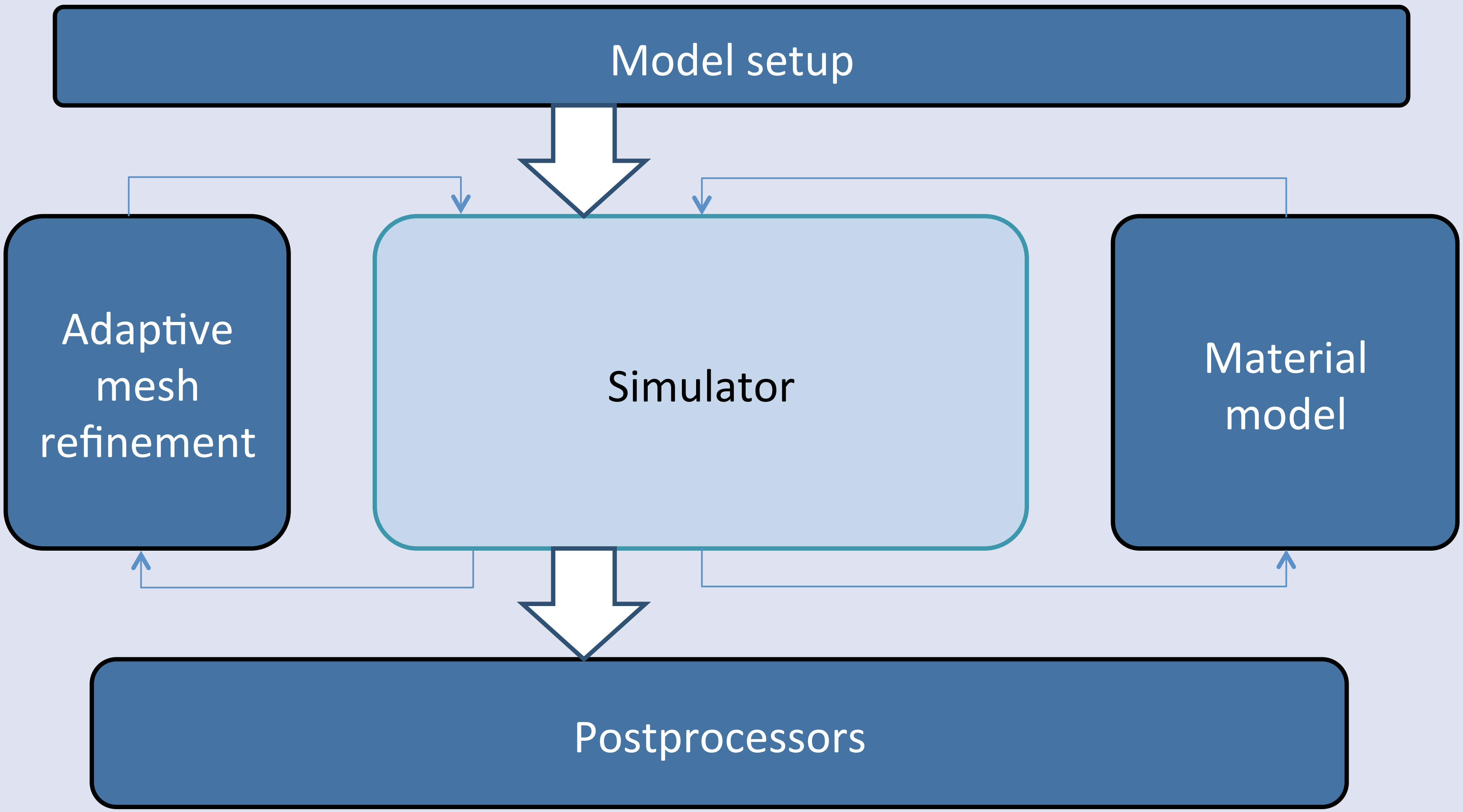
Modularity



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

Modularity



Model setup
Adaptive mesh refinement
Simulator
Material model
Postprocessors

Modularity

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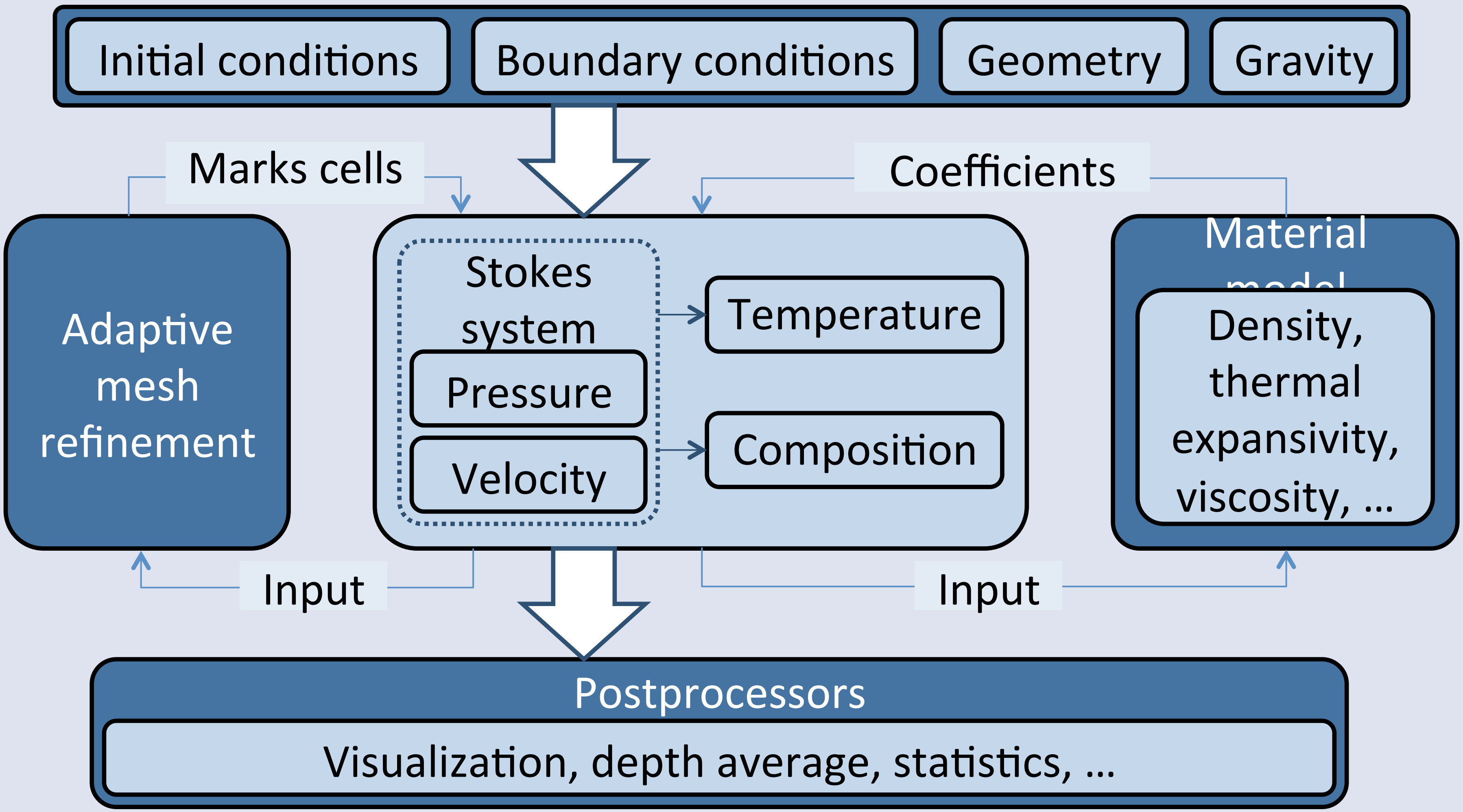

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Checkpointing

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

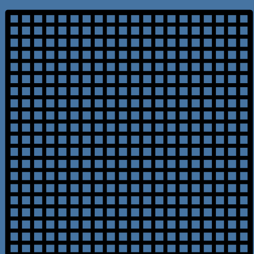
→ Restart required

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

Geometry model

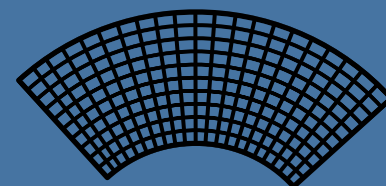
2D or 3D?

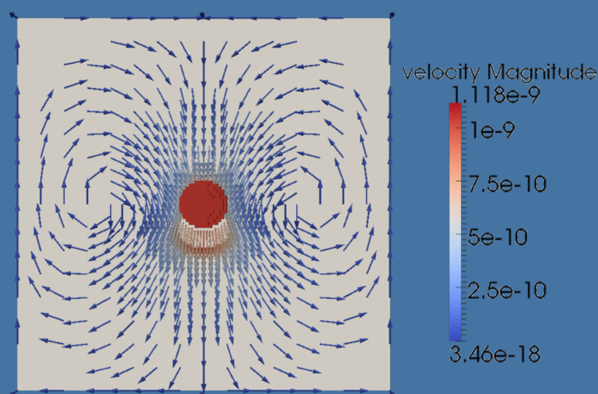
Geometry model

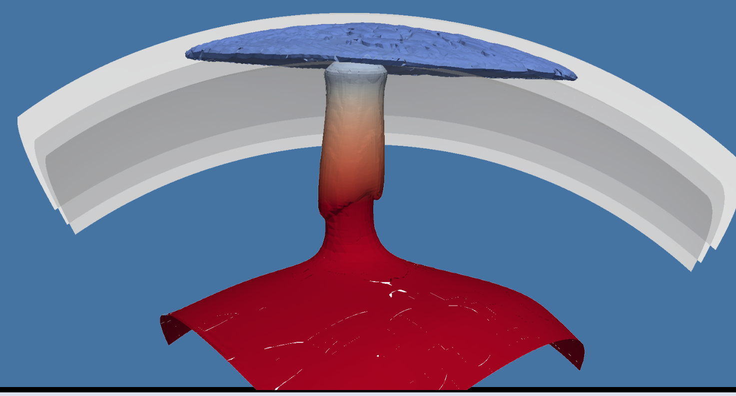


Box

Spherical shell







ASPECT - Discretization

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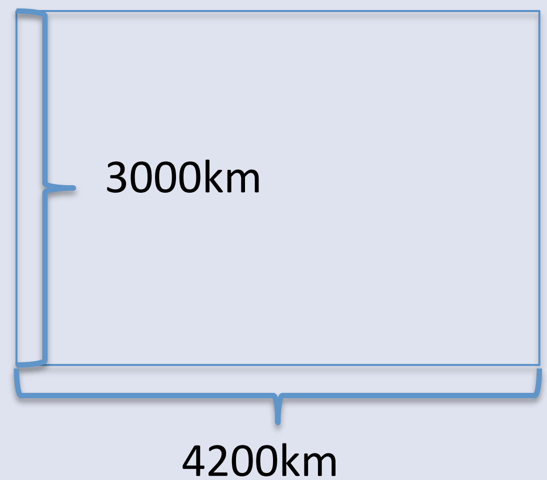
- Aspect has many built in geometry models such as “box” and “shell”.
- A box is a rectangle in 2D and a cuboid in 3D.
- The width (X extent) of the box is 4.2×10^6 meters and the depth (Y extent) is 3×10^6 meters.
- The choice of meters as the unit of length is external to the parameter file; i.e. the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

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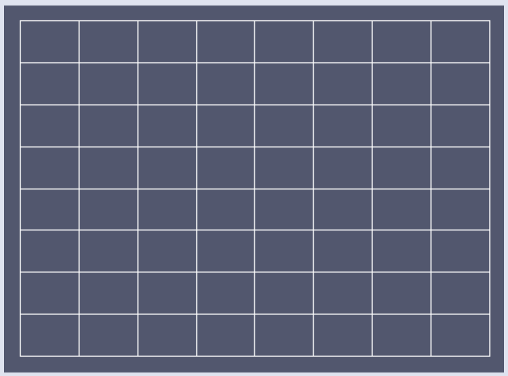
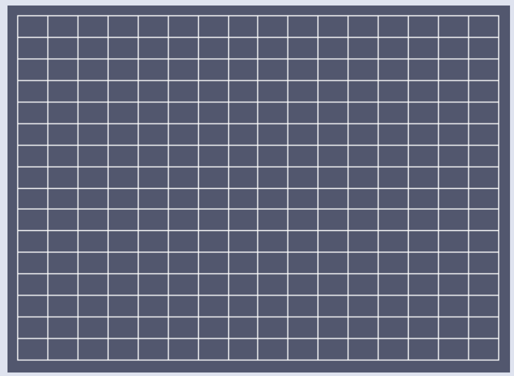
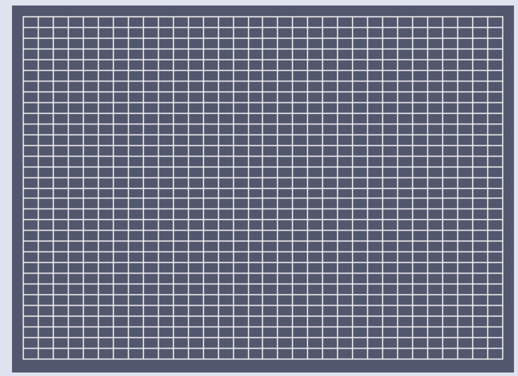
- Initial global refinement specifies the “grid spacing” of our mesh.
- For this tutorial, REFINE=3 or 4 or 5.
- Adaptive mesh refinement has been turned off, i.e. the mesh does not change during the simulation.



REFINE=3 (8x8 cells)



REFINE=4 (16x16 cells)

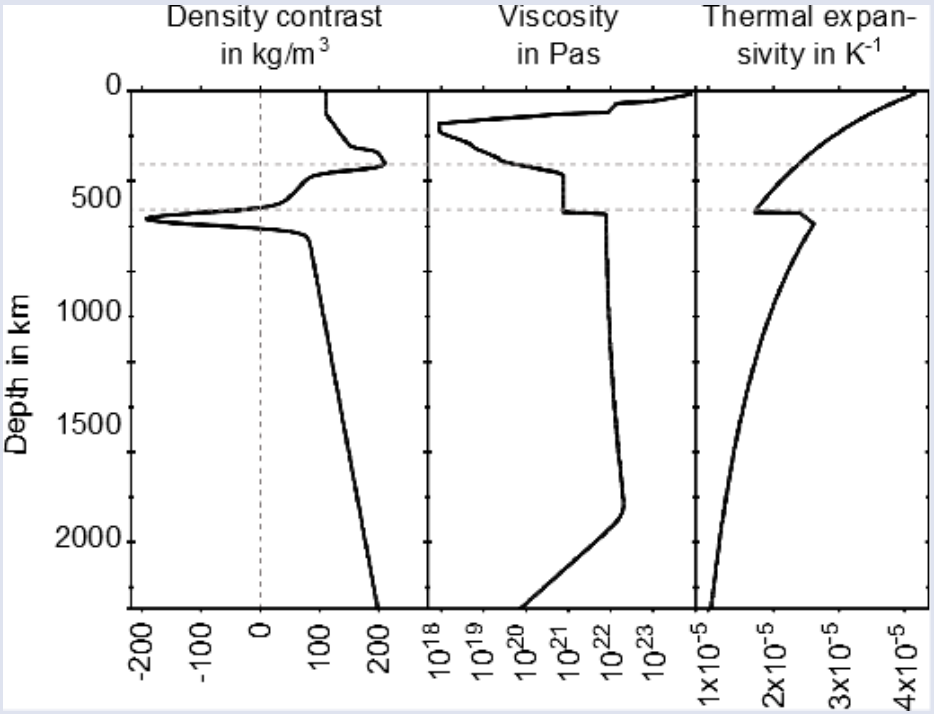


REFINE=5 (32x32 cells)

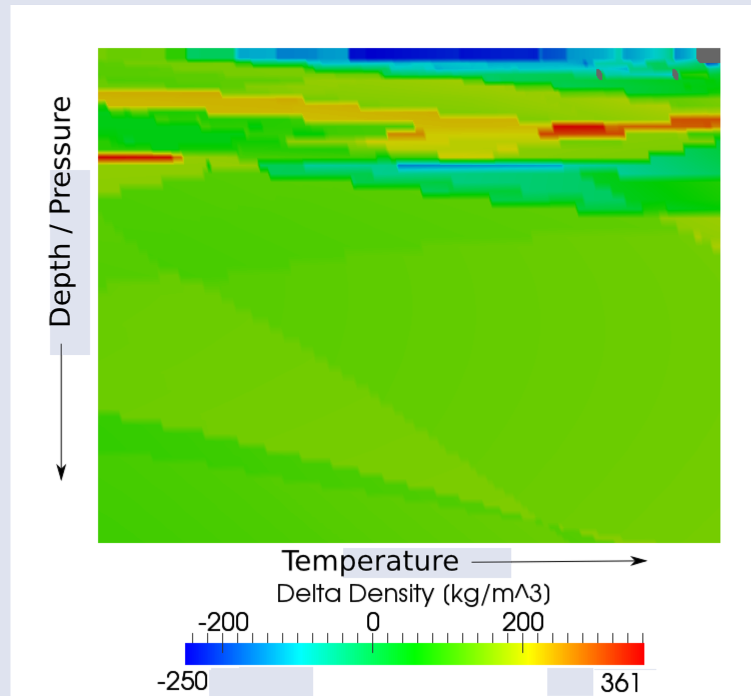
```
subsection Mesh refinement
    set Initial global refinement = REFINE
    set Initial adaptive refinement = 0
    set Time steps between mesh refinement = 0
end
```

Material model

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



Parameterization



Lookup table from Perplex / HeFESTo

ASPECT - Model Parameters

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- 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

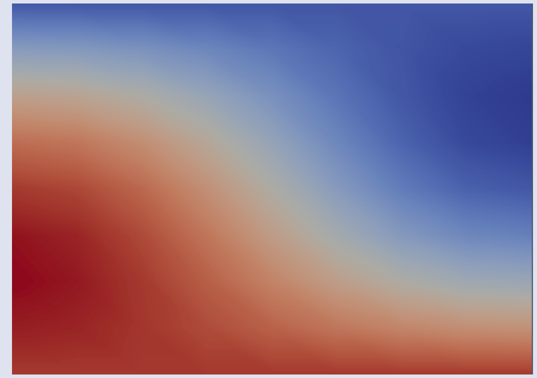
$$\rho_0 = 3300, g = 9.8, \alpha = 2 \times 10^{-5}, \Delta T = (3600 - 273) = 3327$$

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

```
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
```

ASPECT - Initial Conditions



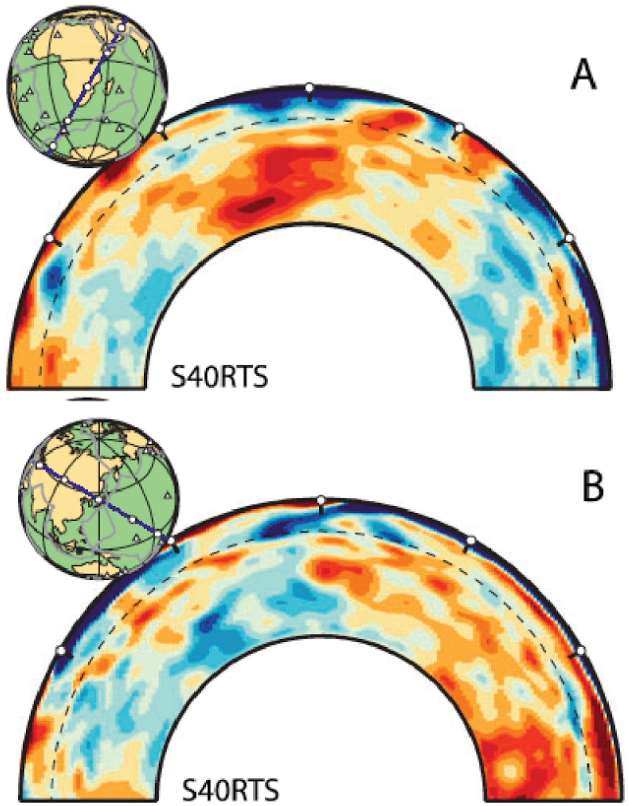
Initial temperature field (p=-0.5)

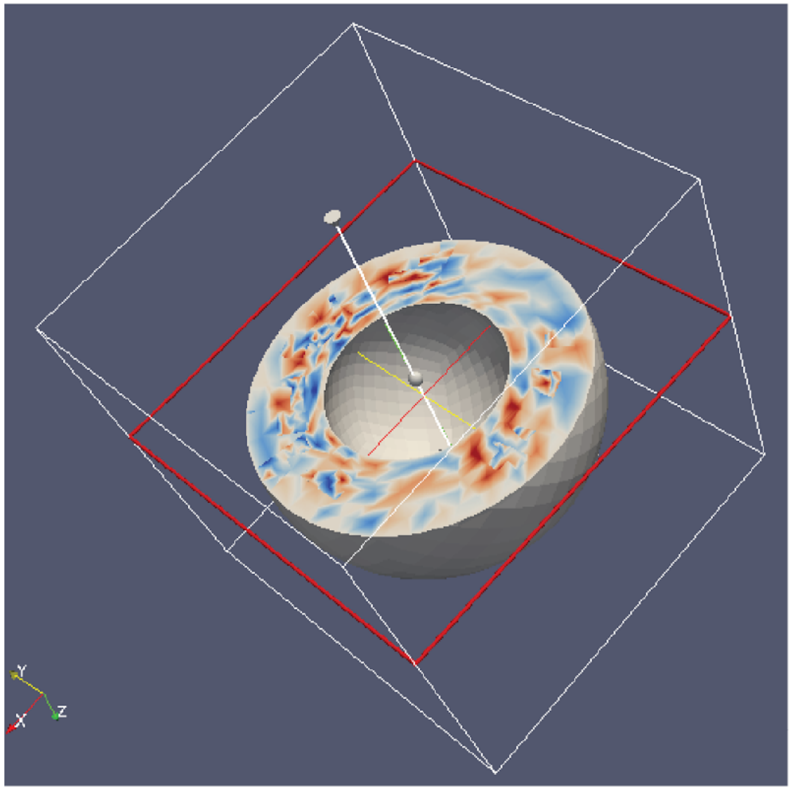
- Aspect has initial condition models to specify the temperature initial conditions and framework for users to implement custom initial condition models.
- The function model lets us specify the initial temperature as a mathematical formula, with user defined constants.
- Here we are specifying a sinusoidal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

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

```
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

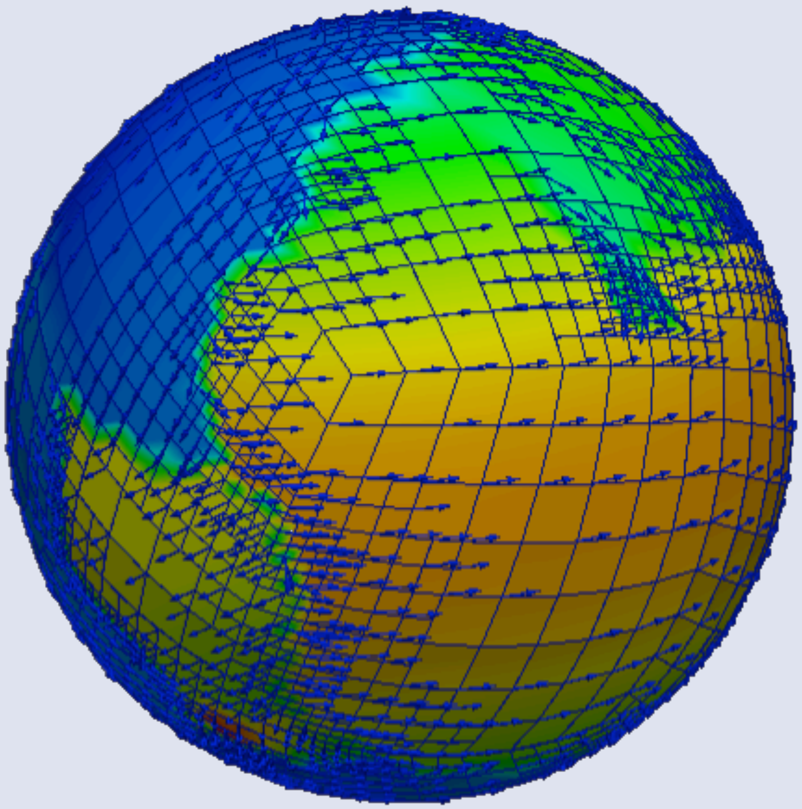
GeoMod2014

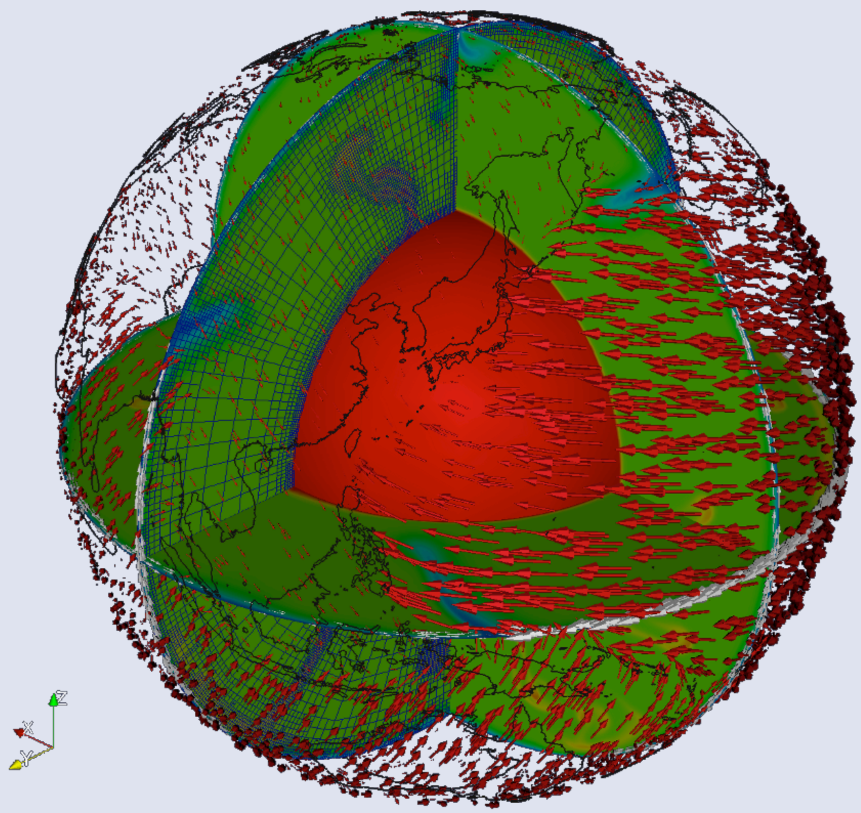
ASPECT - Boundary Conditions

- 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


```
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

GeoMod2014

GPlates

ASPECT - Postprocessing

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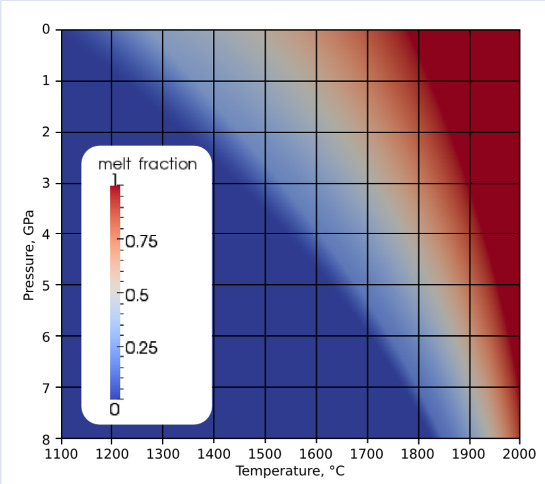
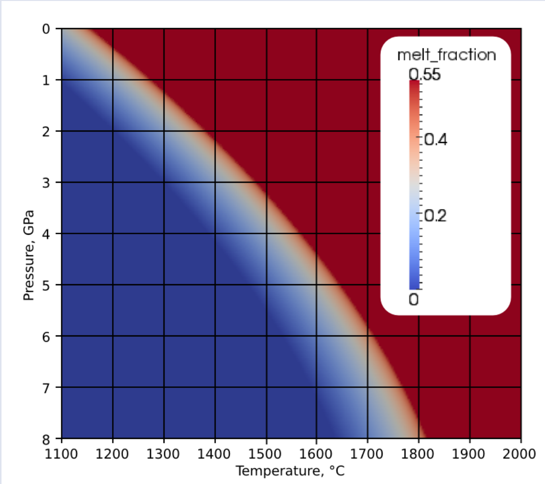
- This section of the parameter file specifies how to analyze the data that has been generated.
- Heat flux statistics and visualization will be used in this tutorial.
- Graphical output is generated every 1e7 simulated years
- We will also add tracer particles to better understand the flow pattern

```
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
```

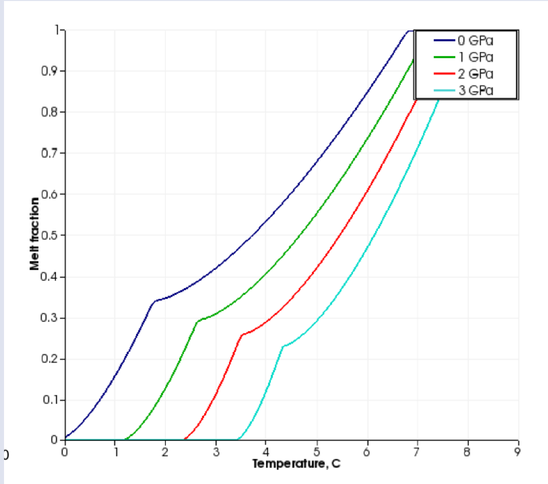
Melt fraction postprocessor

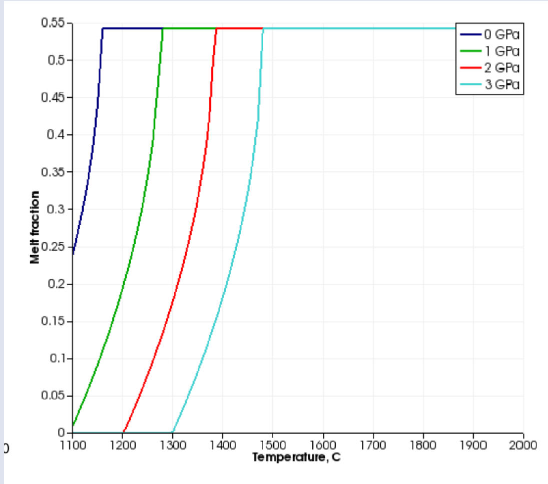
Peridotite
(after Katz et al., 2003)





Pyroxenite
(after Sobolev et al., 2011)





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Latent heat of melting

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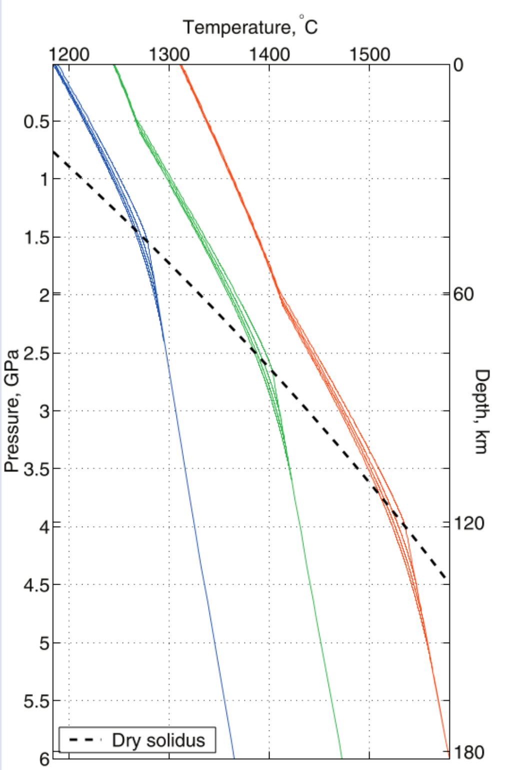
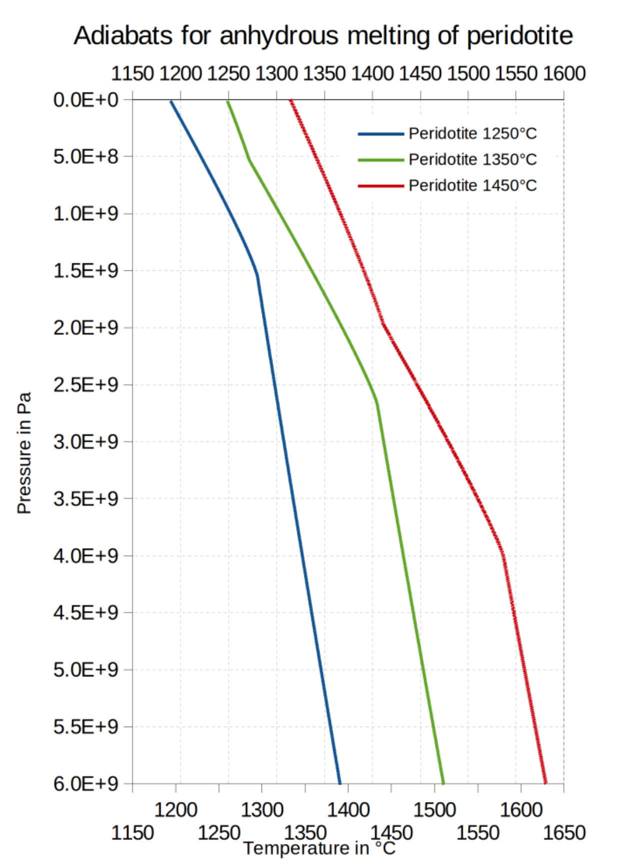
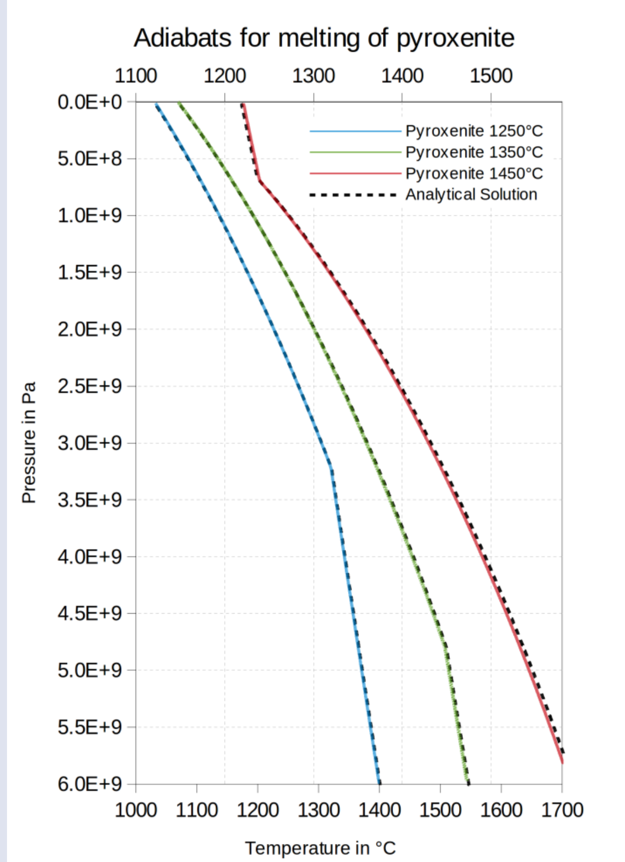
peridotite



From Katz et al., 2003



pyroxenite



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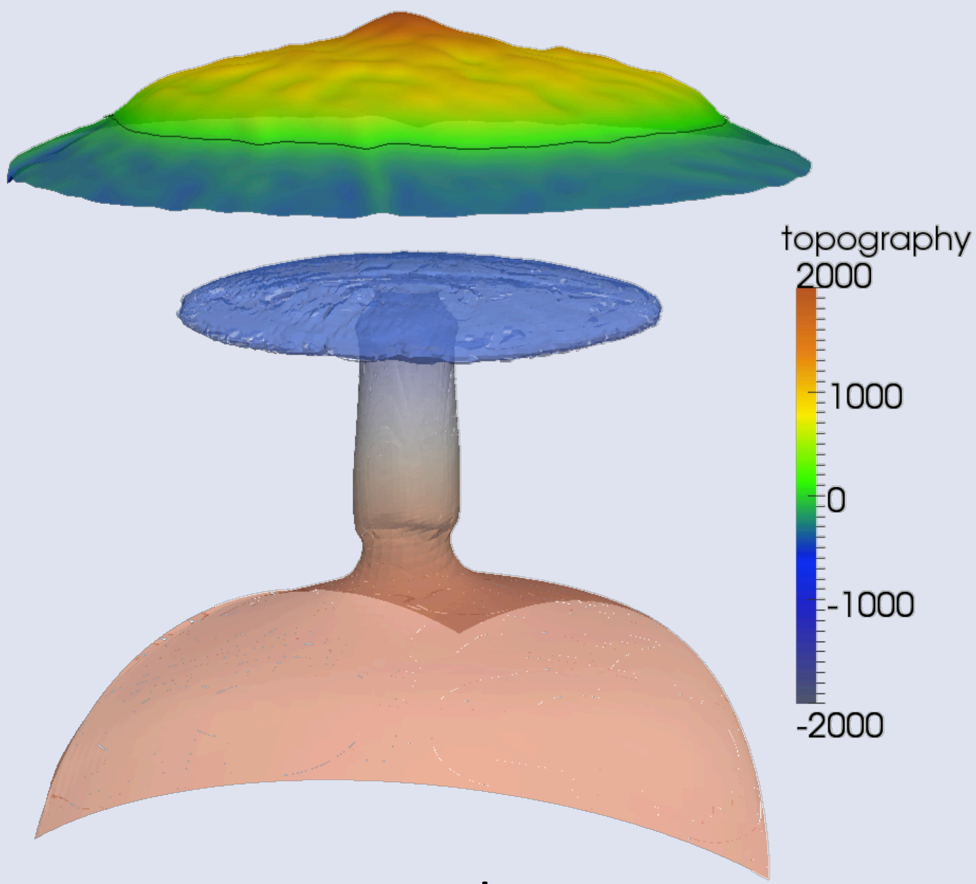
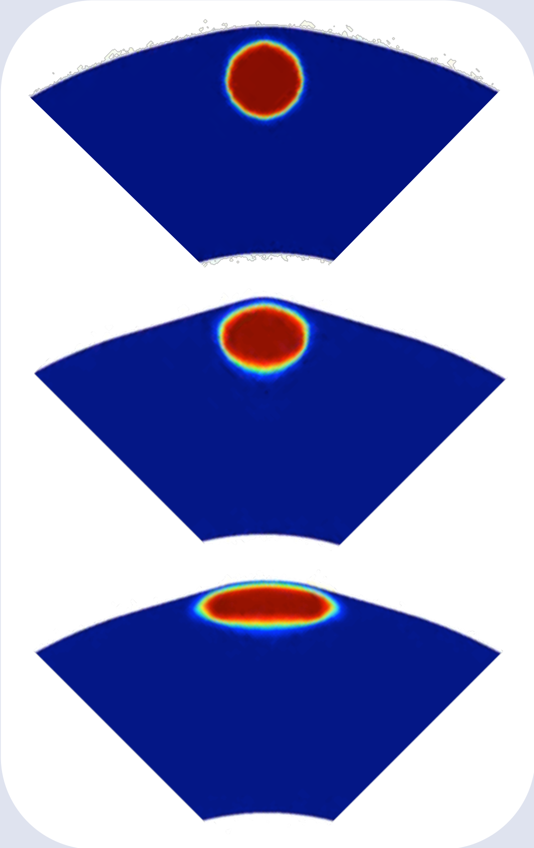
Surface topography



From normal stress



Free surface

From I. Rose

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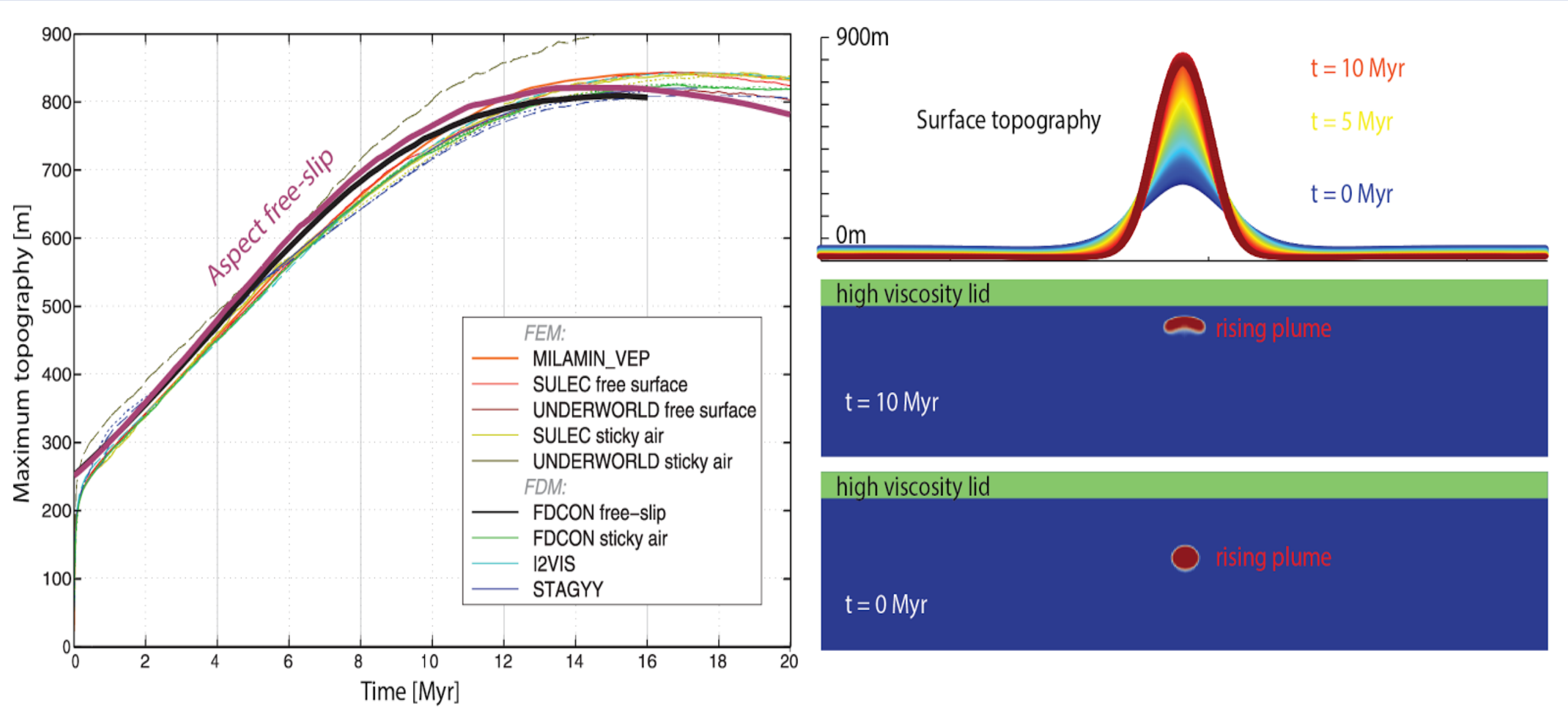
Topography: free-slip (Crameri et al, 2012)



Work with J. Austermann

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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

Tutorial I
Convection in a 2D Box

(Nusselt-Rayleigh Relationship)

GeoMod2014

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 year 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
  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

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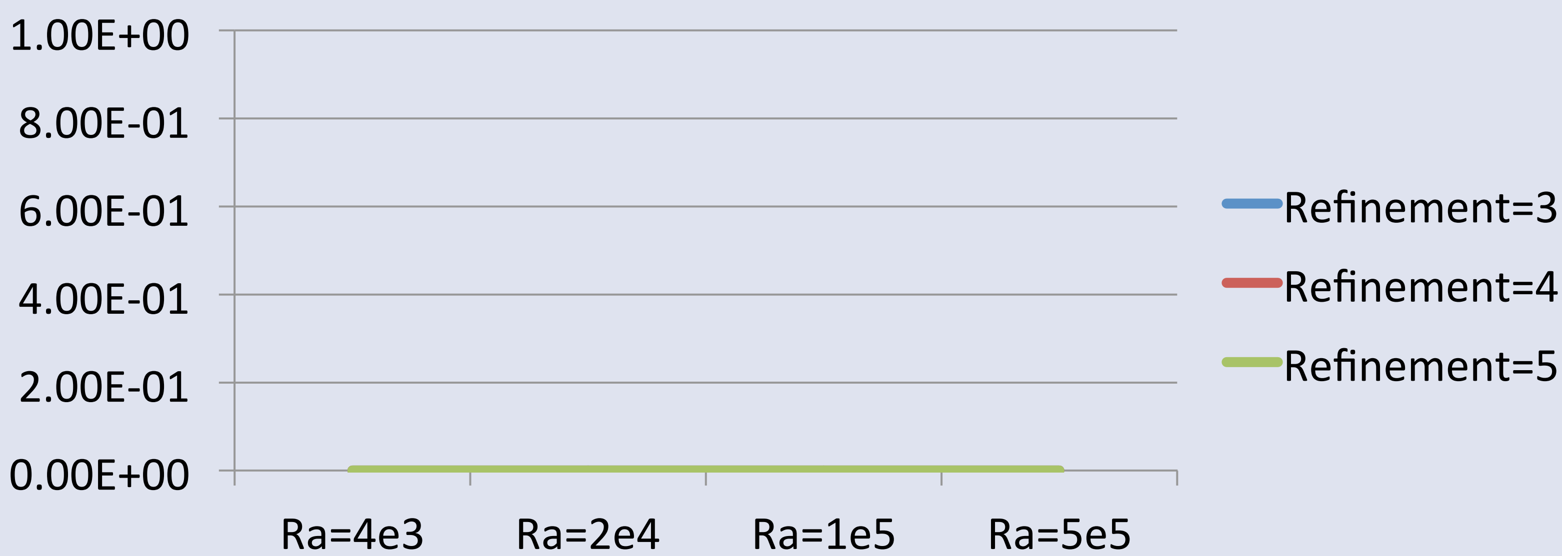
	Ra=4,000	Ra=20,000	Ra=100,000	Ra=500,000
End Time	1e12	2e11	3e10	5e9
Viscosity	1.275E25	2.550E24	5.099E23	1.020E23
Refine = 3	(???)	(???)	(???)	(???)
Refine = 4	(???)	(???)	(???)	(???)



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Nusselt-Rayleigh Answer Key

	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**