COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

Introduction to Numerical Modeling

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Using the Virtual Machine

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- The virtual machine has been tested on Windows, Mac, etc
- We will be showing the same setup on the projector here so you can follow along
- To start, ensure you have VirtualBox and the CIG_VM_CIDER.ova installed

Using the Virtual Machine

- In this tutorial, you will run the programs on a *virtual machine*
- The virtual machine and related programs are on the USB stick we have distributed
- The virtual machine is a program which simulates another computer on your computer
  - This ensures everyone has exactly the same setup, and can follow the tutorial exactly the same way
  - If you want to install ASPECT or other codes on your own machine, please refer to the manual or contact us later for details

Overview

- At the end of this tutorial, you should be able to:
  - Understand why numerical models are used
  - Describe a numerical model and the basic components of it
  - Detail some shortcomings of numerical models
  - Understand basic use of the ASPECT code
  - Edit parameters for an ASPECT simulation
  - Run an ASPECT simulation and analyze the results

Overview

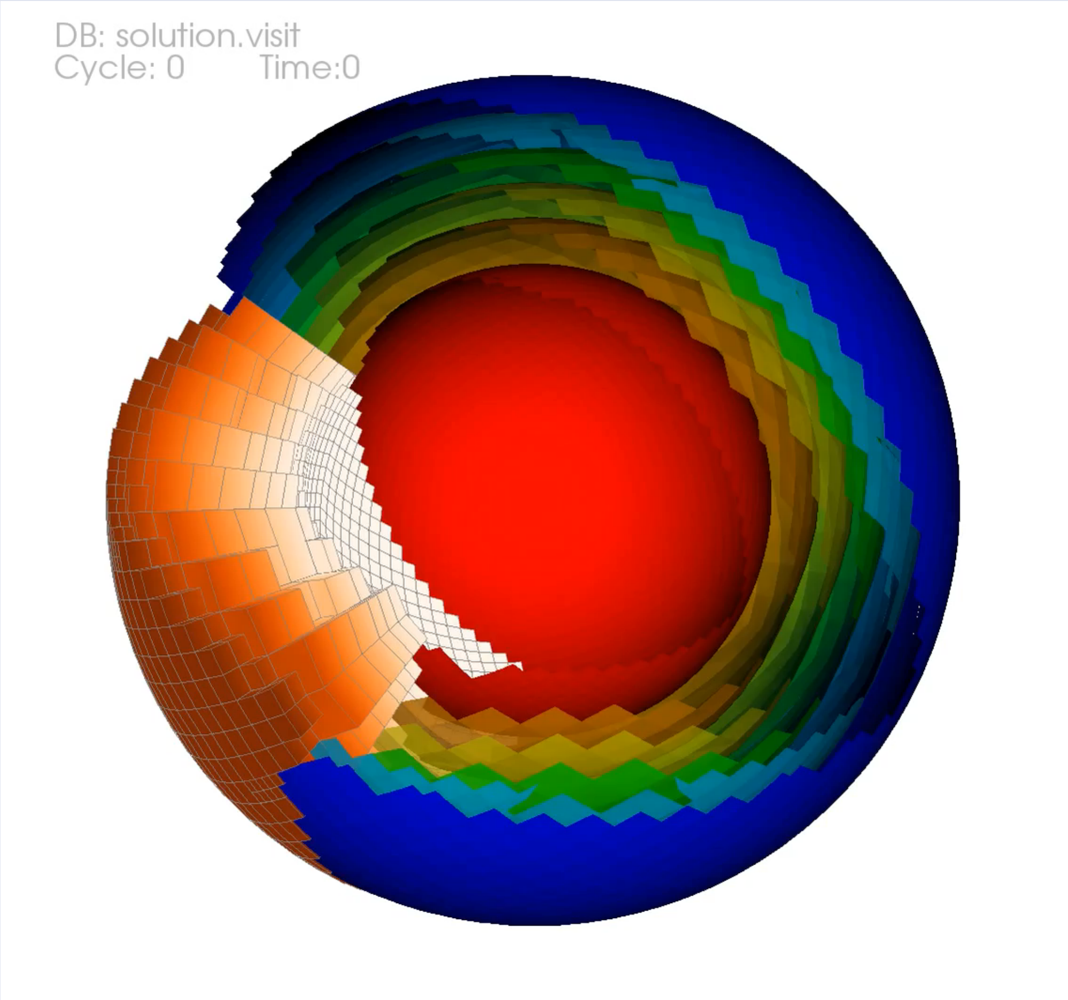
- Why use numerical modeling?
- What is a numerical model?
- Setting up and using the virtual machine
- Numerical modeling with ASPECT
- Modeling the Nusselt-Rayleigh relationship

Why use numerical modeling?

Why use numerical modeling?

- Some phenomenon are too far off experimentally feasible time or space scales
  - Protein folding (10^{-9} meters, 10^{-5} seconds)
  - Galactic evolution (10^{20} meters, 10^{17} seconds)
  - Long term planetary dynamics (10^{6} meters, 10^{16} seconds)
- Since we can't create new universes or planets to study, we model them computationally
- Computational numerical models have successfully been applied in many areas of earth science
- This tutorial will teach you the basics of numerical modeling with a focus towards solid earth science

Why use numerical modeling?

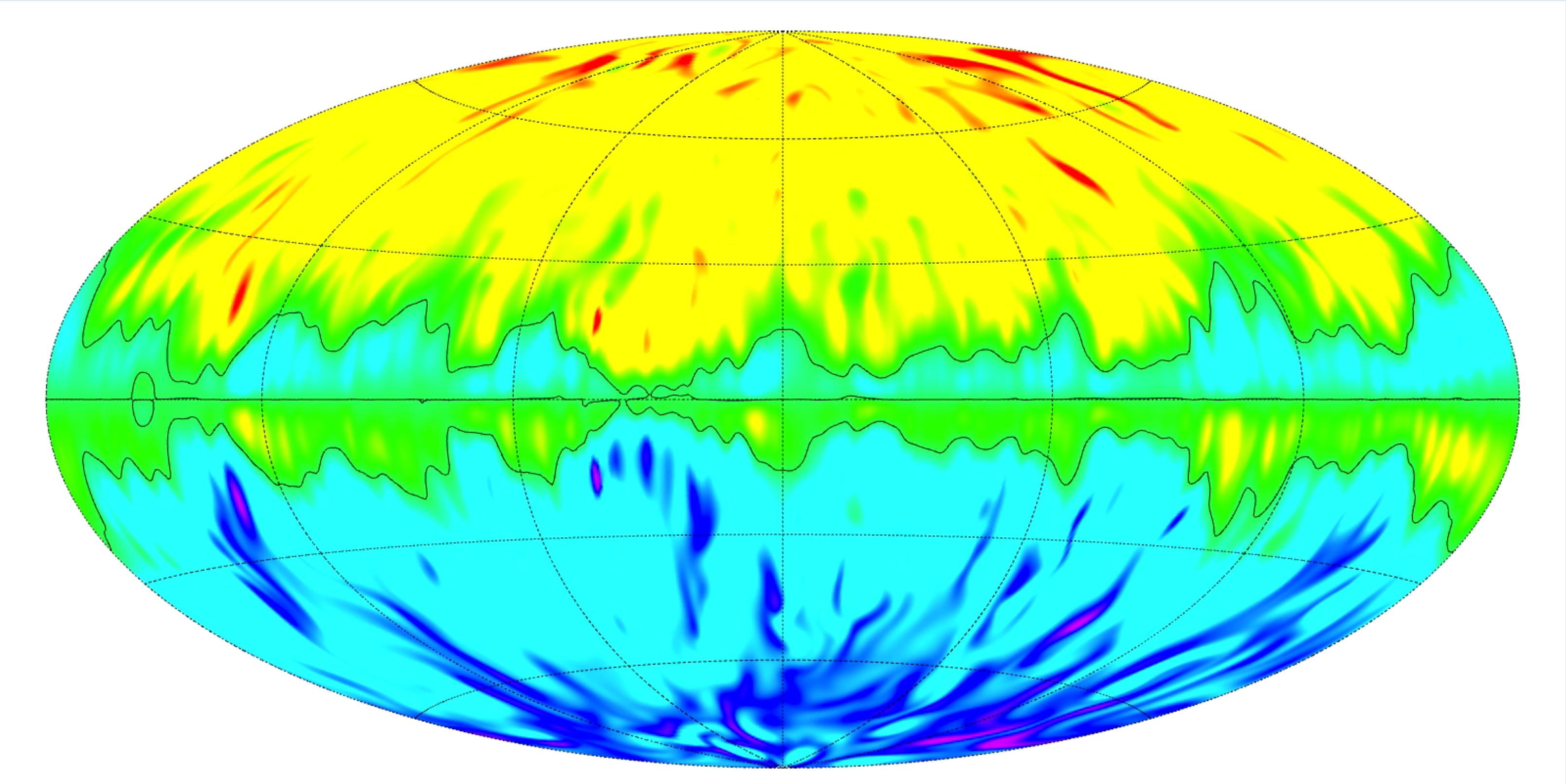


Visualization of simple convection in a spherical shell with ASPECT. Adaptive mesh is shown in the lower left and temperature isosurfaces are shown in the remainder of the shell.

Courtesy Wolfgang Bangerth

Why use numerical modeling?

CIG COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS



Visualization of the radial magnetic field strength at the core mantle boundary from a Calypso simulation.
Courtesy Hiroaki Matsui

Why use numerical modeling?

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- Each of these simulations involved approximations and tradeoffs, for example:
  - Simulation doesn't compute an infinite number of points (lower accuracy)
  - Code doesn't solve equations exactly (makes linear approximations instead)
  - Computers don't represent numbers with perfect accuracy (error creeps into results)
- We will discuss these in more detail later
- Before using numerical models, you must understand these approximations/tradeoffs and how they affect your results

Reality

Simulation

What is a numerical model?

What is a 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

What is a numerical model?

1. The rules (e.g. equations) for the model
   – These are generally partial different equations (PDEs) or ordinary differential equations (ODEs)

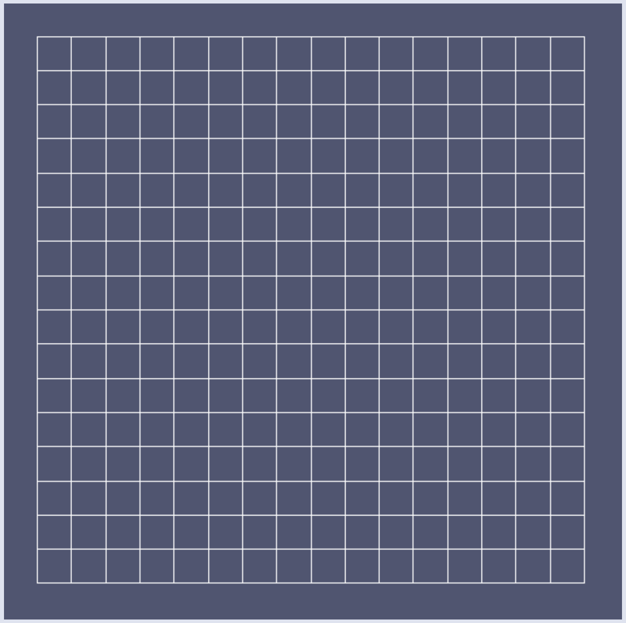
$$\nabla \cdot (\rho \mathbf{u}) = 0$$ Mass conservation

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

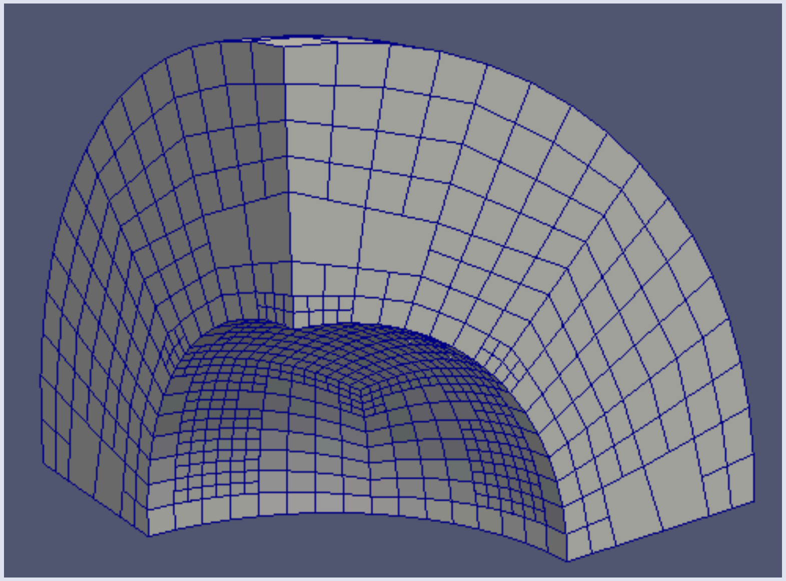
$$F = G\frac{m_1 m_2}{r^2}$$ Gravitational attraction between bodies

What is a numerical model?

2. The discretization of the model
   – Below shows two example meshes with related vertices connected by edges



Simple 2D 17 x 17 vertex
(16 x 16 cell) square mesh



Adaptively refined 3D
quarter shell mesh

What is a numerical model?

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3. Model parameters
   - User controlled values which affect the physics, but do not change during the simulation
   - Examples include material properties, simulation dimensions, physical constants, etc
   - Depending on the code, some values may be parameters in one simulation but dynamic variables in another simulation
     - For example, constant static gravity or dynamically calculated based on actual density field

Parameter	Description
η	viscosity
ρ	density
$\mathbf{g}$	gravity
C_p	specific heat capacity
k	thermal conductivity

Example Parameters

What is a numerical model?

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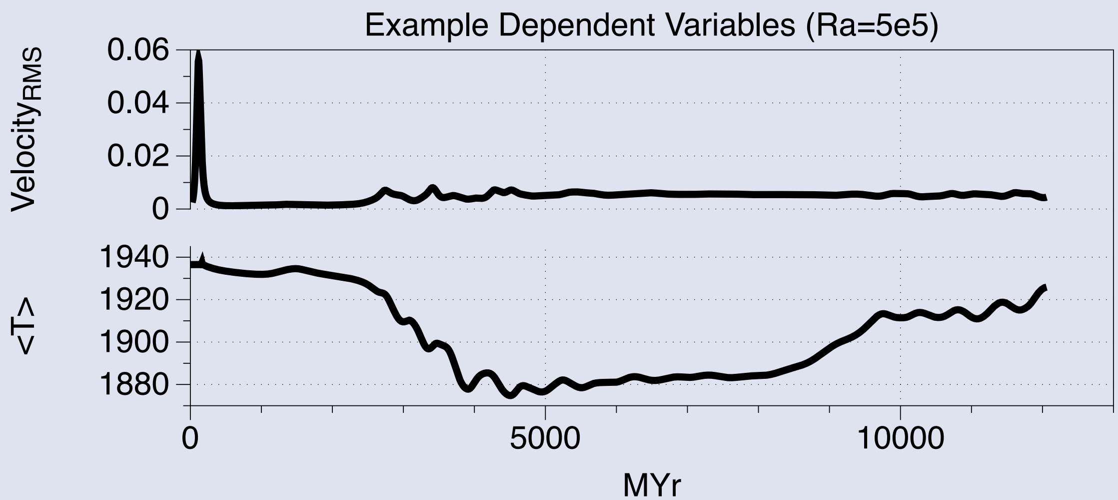
4. Dependent and independent variables
   - Will depend on the equations being solved
   - Independent variables are often related to time and space
   - Examples of dependent ASPECT variables include: temperature, velocity, pressure, density, viscosity, etc



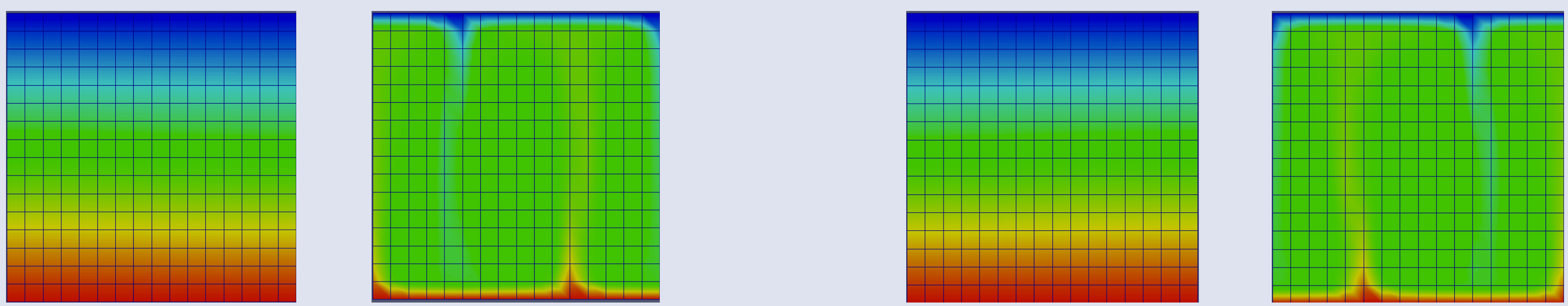
What is a numerical model?

5. The initial state of the model
   - Describes the dependent variables at t=0
   - This can strongly affect results, esp. in a chaotic system
   - Example: initial temperature field in ASPECT

$$T(x,y,t_0) = (1-y) - pcos(\pi x)sin(\pi y)$$

   - Although the perturbation (p) is just 1% of the background, a small change reverses the dynamics

p = 0.01 p = -0.01

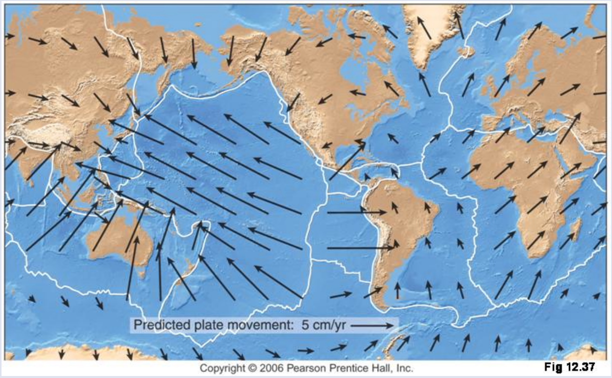


t=0 t=800 t=0 t=800

What is a numerical model?

6. The boundary conditions
   - If the domain isn't infinite, we need to define what happens on the boundaries
   - This must be done for all dependent variables, otherwise the problem is undefined

- Examples
  - Temperature
    - A box with heated bottom, cooled top
    - A mantle with heated interior, cooled exterior
  - Velocity
    - Material can/cannot flow through boundaries
    - Prescribed velocities, possibly matching plate movement (see right)



A map of the velocities predicted for a plate motion model. Plate boundaries are shown in white. (Credit: Pearson Prentice Hall.)

Using ASPECT

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.
  4. Understand the issues regarding the accuracy of simulations.

Using ASPECT

- We will begin by running ASPECT in the Terminal

1. Change to the appropriate directory

```
cd ~/tutorial/aspect
```

2. Run ASPECT with the tutorial parameter file (this will take about 20 seconds)

```
./aspect tutorial.prm
```

3. Open the log and check the Rayleigh number

```
gedit output/log.txt
```

What is a numerical model?

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- 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 - Equations

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

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

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

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

$$+ \frac{\partial \rho}{\partial T} T \mathbf{u} \cdot \mathbf{g}$$ Adiabatic material compression

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

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
```

ASPECT - Discretization

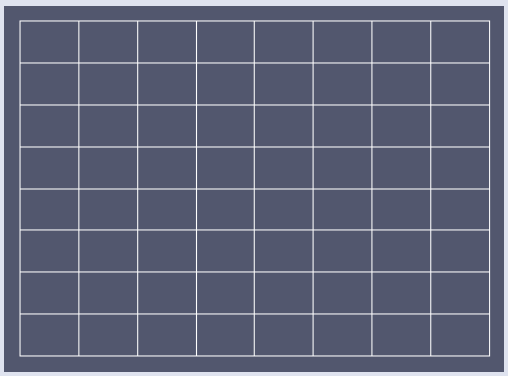
- Aspect has many built in geometry models such as “box” and “shell”.
- A box is a rectangle in 2D and a cuboid in 3D.
- The width (X extent) of the box is 4.2 x 10^6 meters and the depth (Y extent) is 3 x 10^6 meters.
- The choice of meters as the unit of length is external to the parameter file; i.e.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

Simulation Model

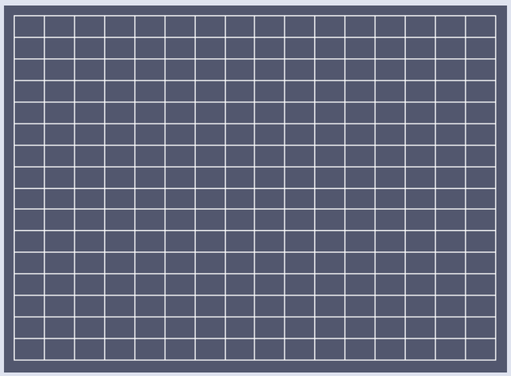

```
subsection Geometry model
    set Model name = box
    subsection Box
        set X extent = 4.2e6
        set Y extent = 3e6
    end
end
```

ASPECT - Discretization

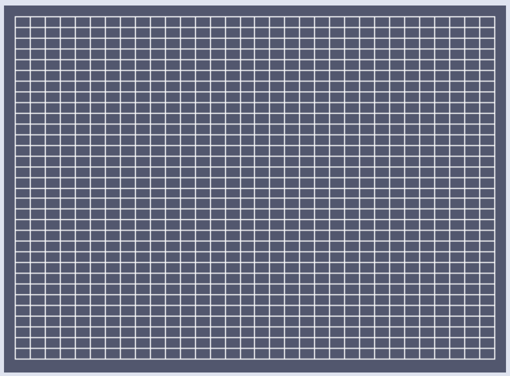
- Initial global refinement specifies the “grid spacing” of our mesh.
- For this tutorial, REFINE=3 or 4 or 5.
- Adaptive mesh refinement has been turned off, i.e. the mesh does not change during the simulation.



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
```

ASPECT - Model Parameters

- 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.

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

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

$$= \frac{5.10452 \times 10^{28}}{Ra}$$

Default Values

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

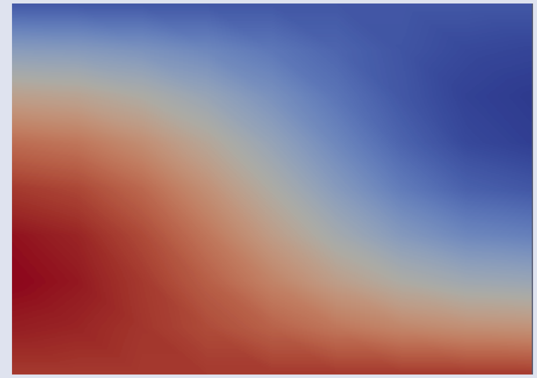
$$D = 3 \times 10^6, k = 4.7, c_p = 1250, \kappa = \frac{k}{\rho_0 c_p} = 1.1394 \times 10^{-6}$$

```
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

- 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
```

ASPECT - Boundary Conditions

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- 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
```

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, visualization, tracers,
        basic 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
```

Visualizing Results with ParaView

Visualization with ParaView

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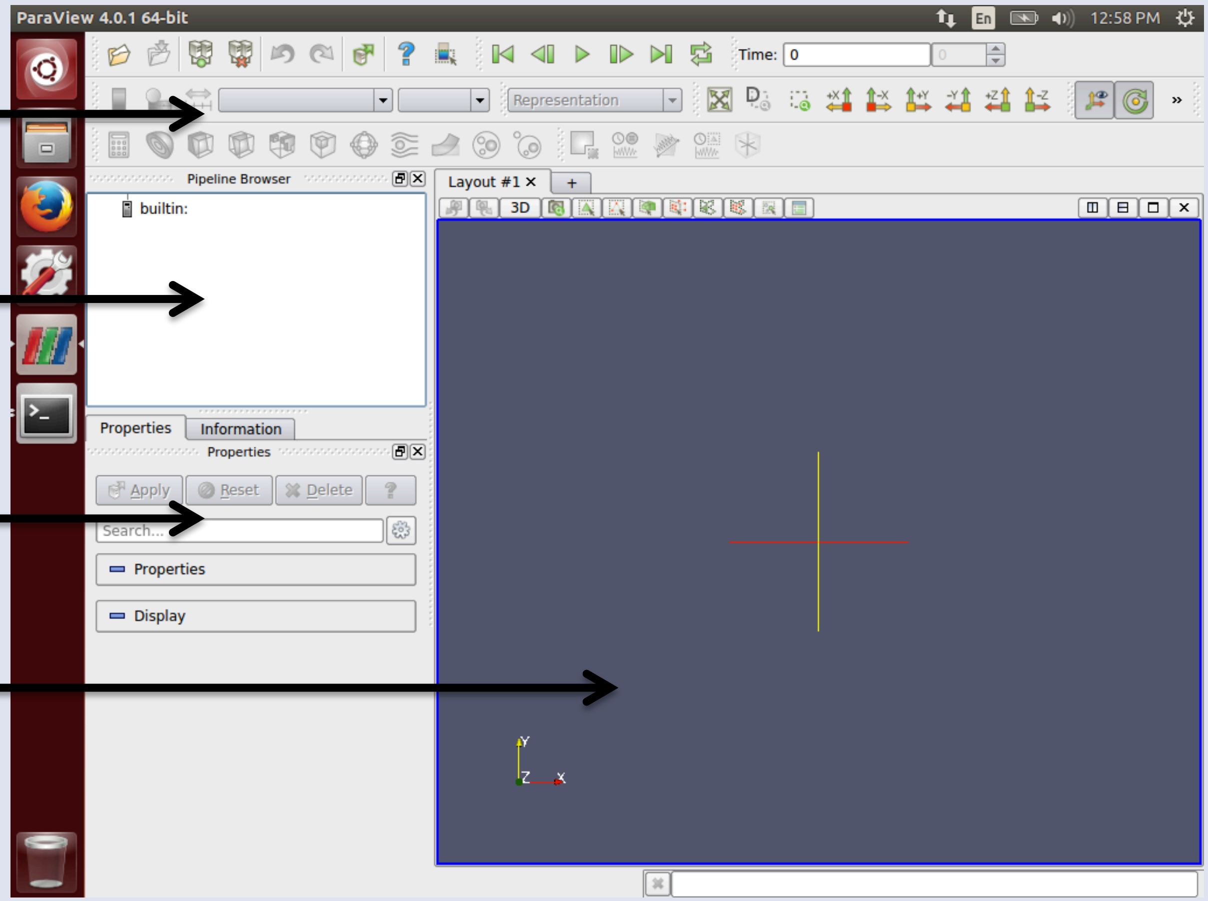
- To visualize the simulation results, we will use ParaView
- ParaView is a program for visualization of large data sets
- It is already installed on the virtual machine, open it now by clicking the icon in the left bar
- ParaView supports visualization tools such as isosurfaces, slices, streamlines,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

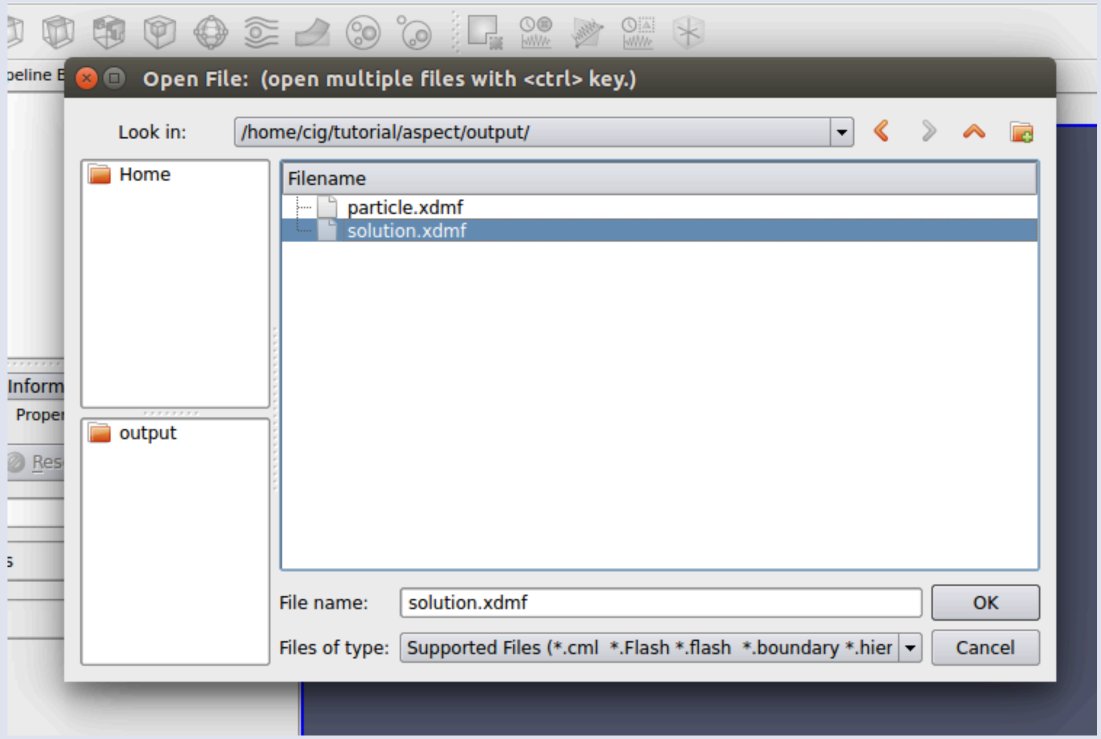
Visualization with ParaView

- Toolbars
- Pipeline Browser
- Object Inspector
- 2D/3D View



Visualization with ParaView

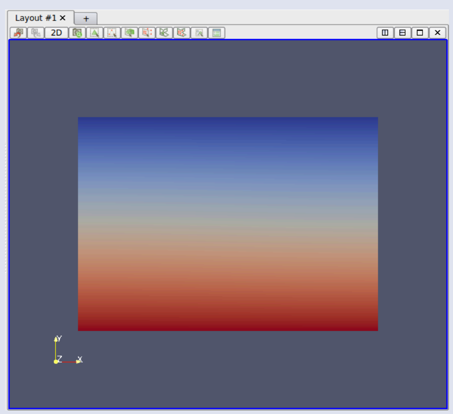
- Start by opening solution.xdmf which was created by running ASPECT

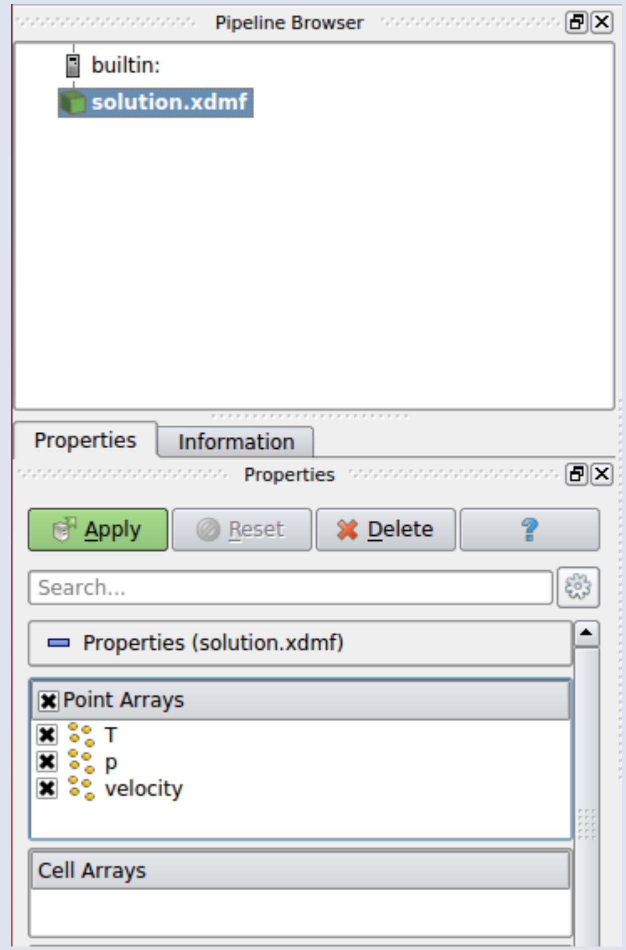


- You can choose "Open" from the File menu or use the Open icon  in the toolbar
- The file is in /home/cig/tutorial/aspect/output/

Visualization with ParaView

- The file will appear in the pipeline browser
  - Make sure this is solution.xdmf
- 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, the temperature field is shown





Visualization with ParaView

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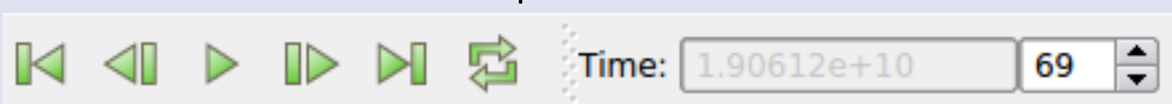
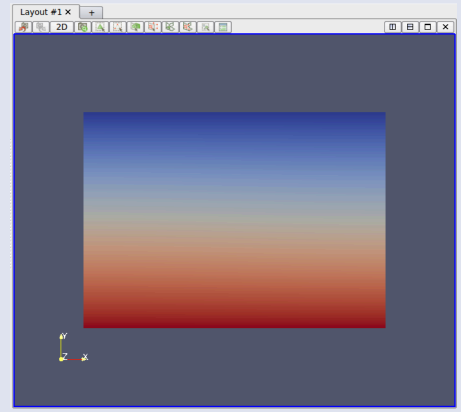
- The top toolbar has buttons to change the time, shown below
  - Click the play button and watch how the temperature field changes
  - Near the end, is the temperature field static? Is the velocity field static? Is material moving?

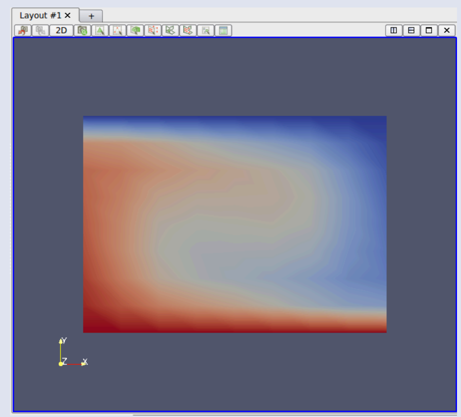
Previous Frame | Next Frame | Loop



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



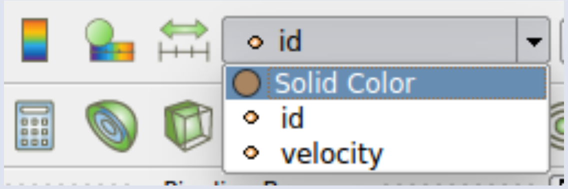
Frame 0



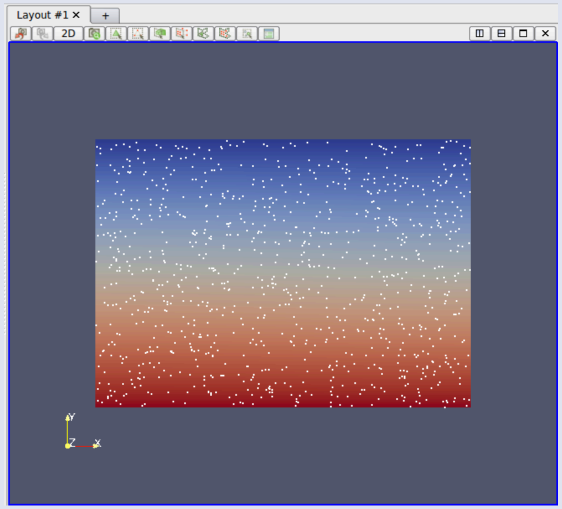
Frame 231

Visualization with ParaView

- Open the file particle.xdmf and click "Apply"
  - The tracer particles from the simulation now appear on the temperature field
  - By default they are colored by ID – change the coloring scheme to "Solid Color" to make them more visible
  - 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

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 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

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- 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
  2. Run the simulation
  3. Visualize the results and make sure they are realistic
  4. Calculate the Nusselt number from the heat flux

$$Nu = \frac{\frac{Q}{L}}{\frac{k\Delta T}{D}} = \frac{\frac{Q}{4.2e6}}{\frac{4.7(3600-273)}{3e6}} = \frac{Q}{21892}$$

Nusselt-Rayleigh Relationship

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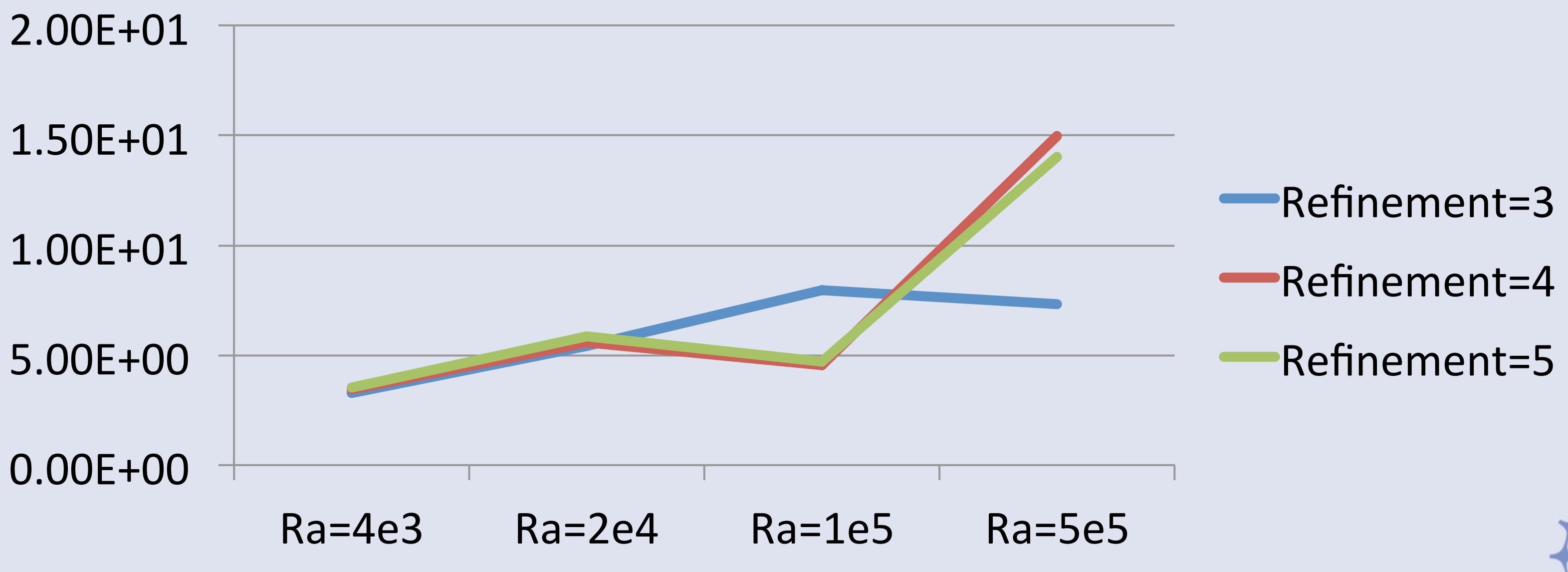
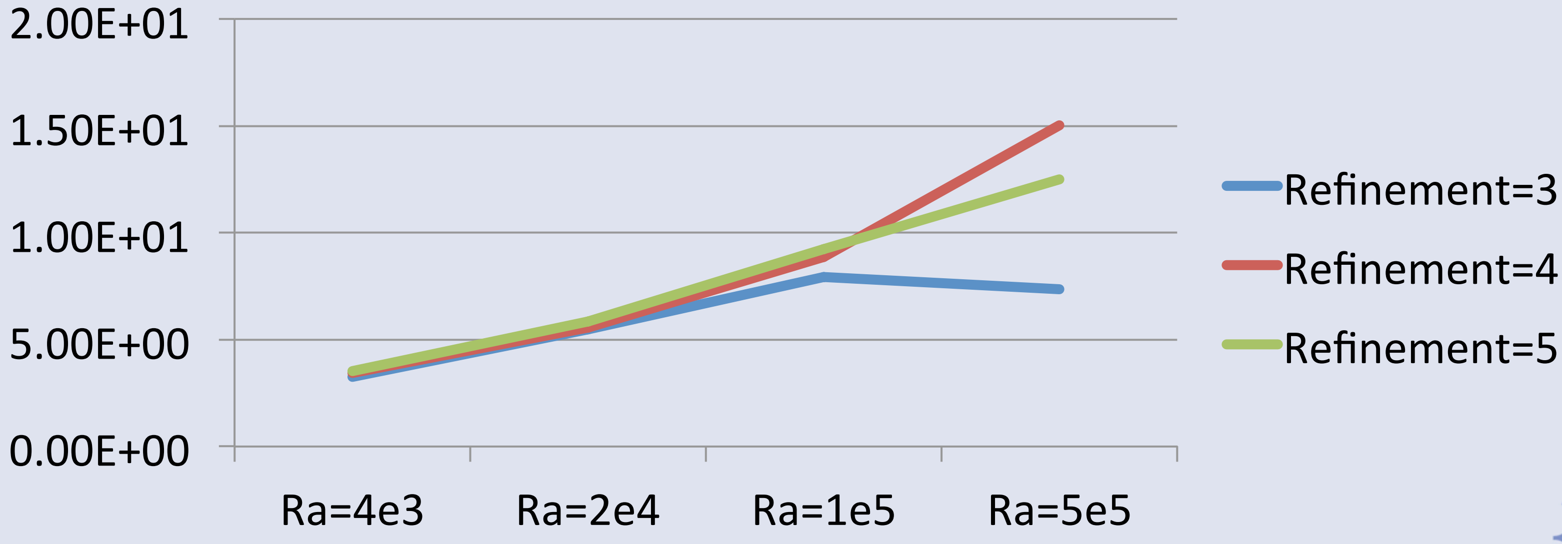
	Ra=4,000	Ra=20,000	Ra=100,000	Ra=500,000
End Time	2e11	5e10	3e10	1e10
Viscosity	1.275E25	2.5522E24	5.1045E23	1.0209E23
Refine = 3	3.269	5.436	(???)	7.308
Refine = 4	3.43	5.59	4.567	14.98
Refine = 5	(???)	5.86	4.7	(???)



Nusselt-Rayleigh Answer Key

	Ra=4,000	Ra=20,000	Ra=100,000	Ra=500,000
End Time	2e11	5e10	3e10	1e10
Viscosity	1.275E25	2.5522E24	5.1045E23	1.0209E23
Refine = 3	**3.26**	**5.48**	**7.95**	**7.36**
Refine = 4	**3.45**	**5.57**	**8.86**	**14.99**
Refine = 5	**3.53**	**5.85**	**9.23**	**13.94**
R=3, R=5 Diff	**8.3%**	**6.8%**	**16.1%**	**89.4%**



Nusselt-Rayleigh Relationship

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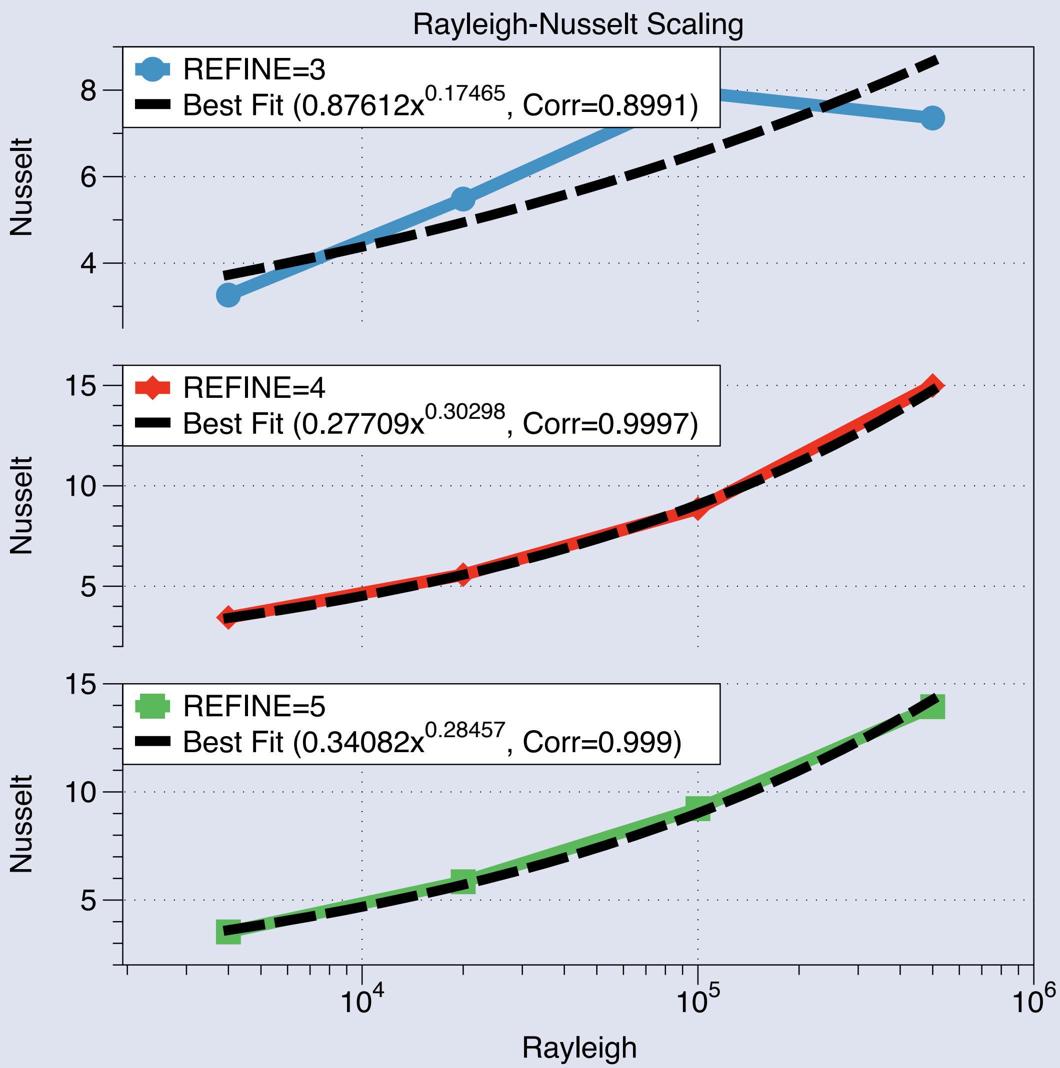

- As the Rayleigh number increases, higher refinement is needed to correctly resolve the problem
- Standard measurements of Ra-Nu relationship show a power-law relationship Nu=a(Ra^b) where b is between 0.25 and 0.35