Geodynamic modeling with ASPECT

Laurent Montesi

Following tutorials by Eric Heien (CIDER 2014)
and Juliane Dannberg / Rene Gassmoller (Geomod 2014)
With help from CIG
Bill Broadley, Tyler Esser, Lorraine Hwang, and Louise Kellogg

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

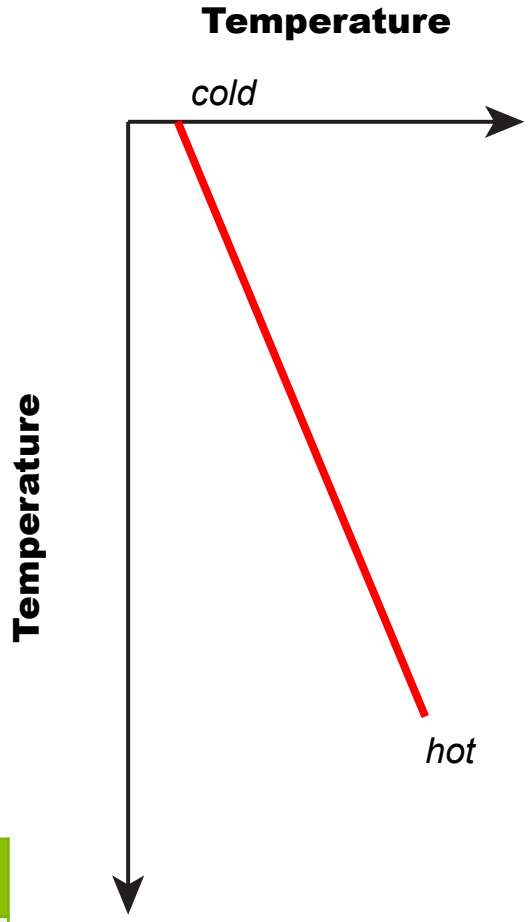
Tutorial Objectives

- Understand better numerical modeling
- Learn basic use of the ASPECT code
  - Command line operations
  - Equations for mantle convection
- Edit parameters for an ASPECT simulation
  - Boundary conditions
  - Grid refinement
- Visualize ASPECT output using Paraview
- Analyze ASPECT simulation results
  - Document the Nusselt-Rayleigh number relation

Nusselt what?

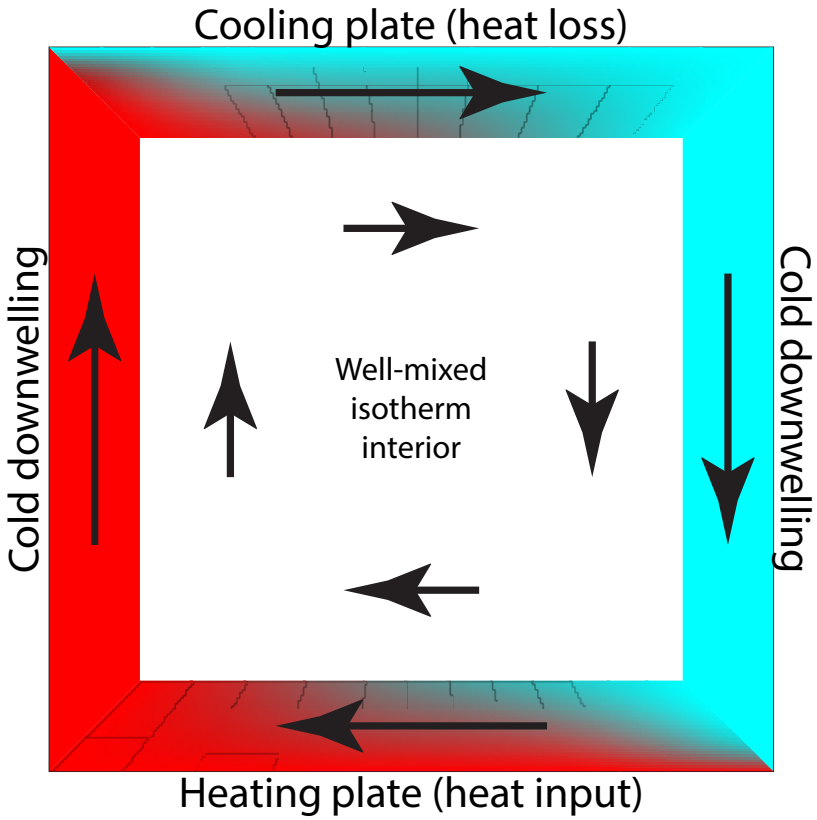
- Box heated from below. Static solution is a linear temperature gradient
- Hot material is low density => unstable statification
- Conductive heat flux

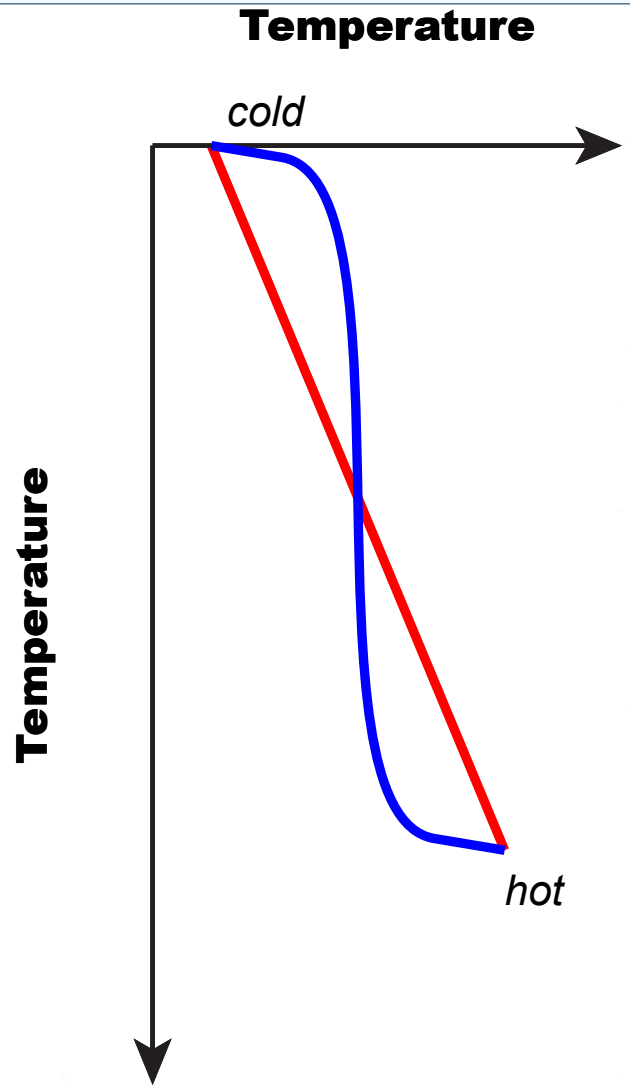
$$q = k\frac{\Delta T}{D}$$



q	k	ΔT	D
Heat flux	Thermal conductivity	Temperature change	Thickness

Convection intensifies heat flux





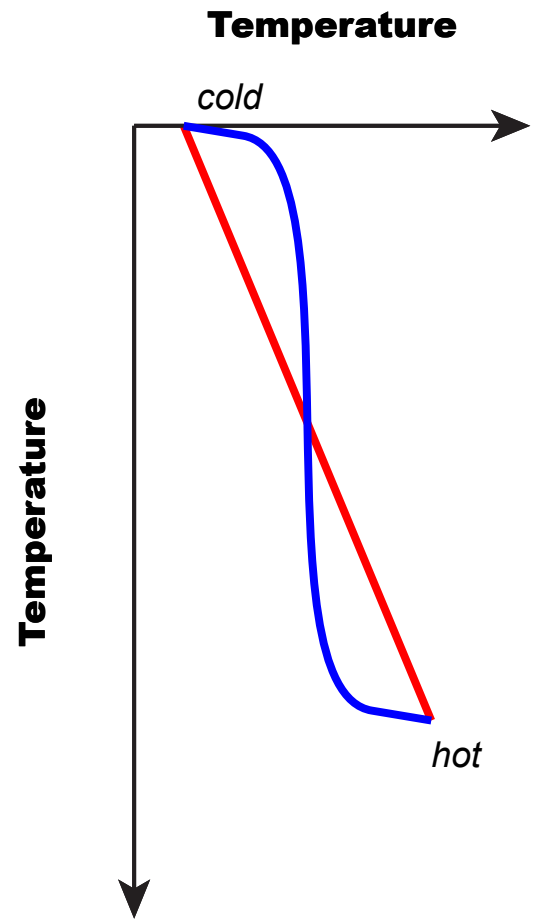
Nusselt what?

- Hot, low density material wants to rise.
- If viscosity is low enough: convection!

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

- Hot material near the surface generates high heat flux (boundary layer)

$$\mathrm{Nu} = \frac{q}{k \Delta T / D}$$



ρ_0	g	α	ΔT	D	η	κ
Density	gravity	Expansion coefficient	Temperature change	Thickness	viscosity	Thermal diffusivity

How is modeling useful?

- Simulate processes that take place at length scales and temporal scales inaccessible to direct observation.
- Simplify a natural system to a well-controlled set of basic principles (physical, chemical, or otherwise)
- A model will not reproduce reality exactly. Its utility is in reveal fundamental relations between basic principles and a range of observations
- Models can be conceptual, analog, analytical, or numerical

When is numerical modeling useful?

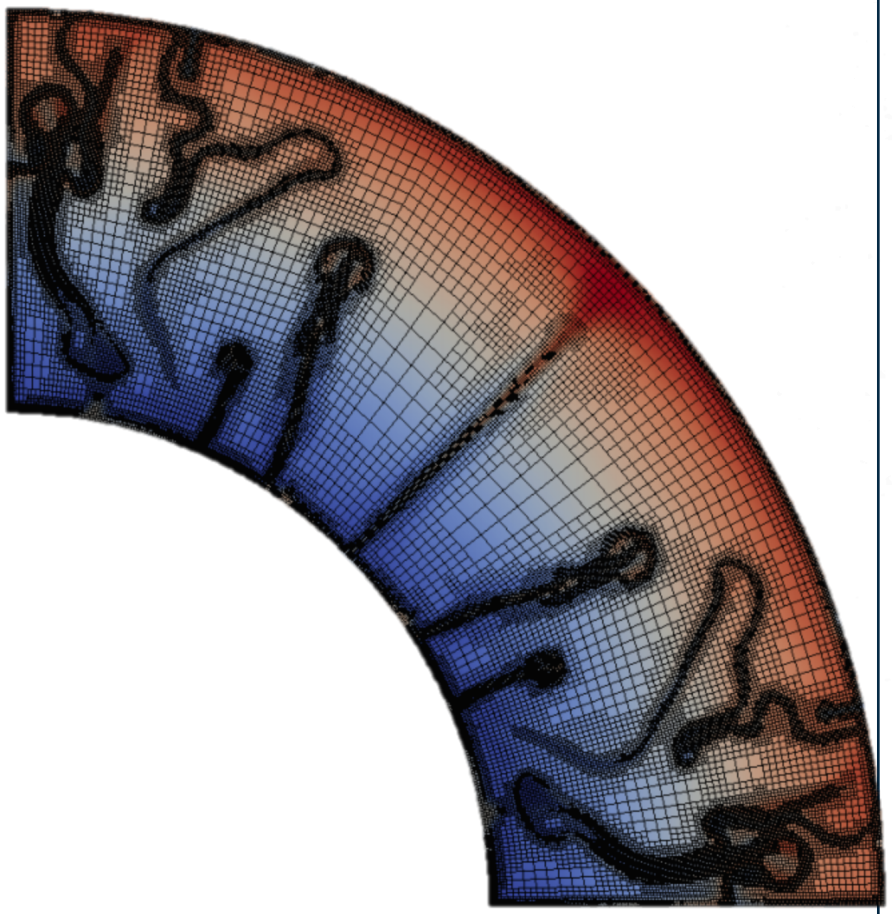
- Systems to large or too complex for modeling by other means
- Computer modeling is designed to save the user time, but typically rely of approximation that may or may not modify system behavior
- No code solves the underlying system exactly
  - Discretization of the system of equations and/or space
  - Linear approximation to coupled equations
  - Rounding errors (numbers are truncated; errors can accumulate)

What's in a numerical model?

- Physics
  - Equations to solved (conservation of mass, momentum, energy)
  - Model parameters and constitutive relations (thermal conductivity, viscosity)
  - Model geometry (one or two layers?)
  - Boundary conditions (free slip, no heat flux, prescribed temperature)
  - Initial state of the model (Material at rest, uniform temperature)
- Numerics
  - Discretization strategy (Finite Element method)
  - Solver (how to solver the system of equations)

ASPECT

- Advanced Solver for Problems in Earth's ConvecTion
- Developed by CIG by Wolfgang Bangerth, Timo Heister, and many others
- Guiding principles:
  - Usability and extensibility
  - Modern numerical methods
  - Parallelism
  - Building on other's work
    - deal.II and many other packages
  - Community
    - Annual Hackathon
    - Open-source



Conservation equations in ASPECT

- Mass conservation $\nabla \cdot (\rho \mathbf{v}) = 0$
- Momentum conservation $-\nabla \cdot \left\{ 2\eta \left[\dot{\varepsilon} - \frac{1}{3}(\nabla \cdot \mathbf{v})\mathbf{I} \right] \right\} + \nabla P = \rho \mathbf{g}$
- Heat conduction

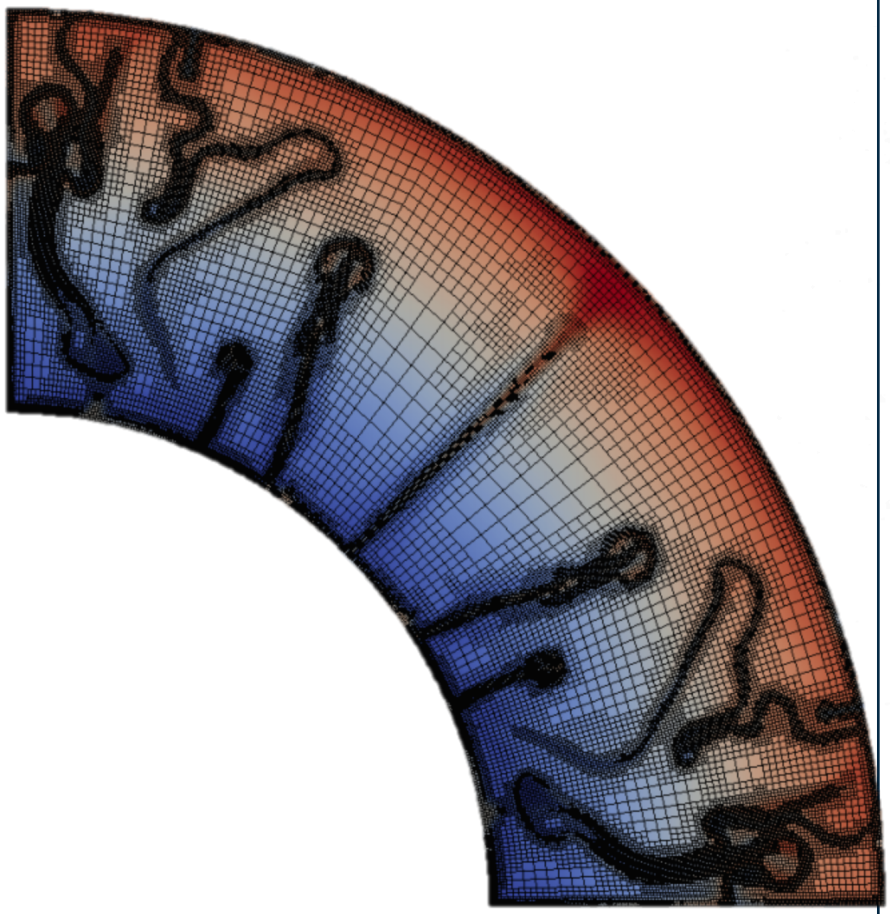
$$\rho C_p \left(\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) - \nabla \cdot (k \nabla T) = \rho H + \frac{\partial \rho}{\partial T} T \; \mathbf{v} \cdot \mathbf{g} + 2\eta \left[\dot{\varepsilon} - \frac{1}{3}(\nabla \cdot \mathbf{v})\mathbf{I} \right] : \left[\dot{\varepsilon} - \frac{1}{3}(\nabla \cdot \mathbf{v})\mathbf{I} \right]$$

$\mathbf{v}$	Velocity	m/s
P	Pressure	Pa
T	Temperature	K
$\dot{\varepsilon} \equiv \frac{1}{2}(\nabla \mathbf{v} + \nabla \mathbf{v}^T)$	Strain rate	s^{-1}
η	Viscosity	Pa s

ρ	Density	Kg/m^3
$\mathbf{g}$	Gravity	m/s^1
C_p	Heat capacity	J/kg/K
k	Heat conductivity	W/m/K
H	Heat production	W/kg

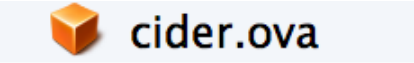
Aspects of ASPECT

- Finite Element method
- Tracer particles
  - Can carry composition, history-dependent state variables
- Adaptive mesh refinement
  - More efficient for 3-D problems
  - "Follow" interesting localized features, e.g. slabs, plumes, faults
  - Arbitrary Lagrangian-Eulerian formulation
    - Free surface, large deformation
  - New developments: plasticity, melt migration
- Limits
  - Set of pre-defined shapes
  - Software dependencies
    - MPI, Trillinos, p4est, deal.II,



Starting Virtual Machine

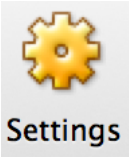
- You should have downloaded the VirtualBox software from https://www.virtualbox.org/wiki/Downloads and the virtual machine image from https://wiki.geodynamics.org/software:aspect:cider_2015.

- Open VirtualBox
- In the File menu, select Import Appliance
- Click on the yellow folder and browse to wherever you saved the 

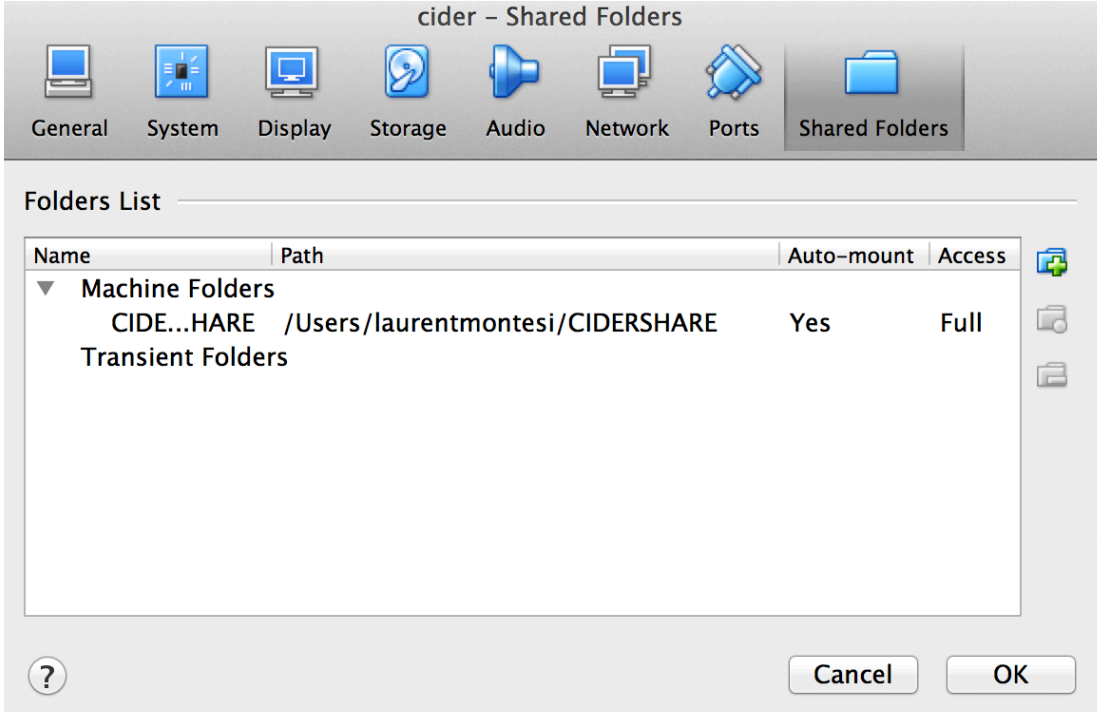
appliance

Setup a shared folder

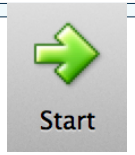
- **Optional but useful** in other tutorials to transfer documents from the virtual machine to your native operating system
- Before starting the VM, click settings



- Click Shared Folders
- Click the folder with a + sign to select a folder on your native system (macOS or windows)
- Click OK



Shared folder (cont'd)

- Start the Virtual Machine 

(close the warning messages)
- When the VM is up, open a Terminal window 
- You need to install an extension
  - Type `sudo apt-get update && sudo apt-get install dkms`
  - Wait until the command suceeds, then Go to the top bar menu and under Devices at the bottom of the list, click: **Insert Guest Additions CD Image**
  - A window may pop up asking to run the CD. Hit 'cancel'.
  - In the same terminal as before, type: `cd /media/cig/VBOXADDITIONS`' and then use the tab key to autocomplete. If it autocompletes, hit enter.
  - Now, type: `sudo sh ./VBoxLinuxAdditions.run`
- Restart the VM and reopen a terminal window.
  - The shared directory in the VM is at /media/sf_<sharename> where <sharename> is the name of the directory you chose in your native OS.
  - Optional: Make a symbolic link to find it easily. In the terminal window, type `ln –s /media/sf_<sharename> ~/<sharename>`

Initializing ASPECT

- Open parameter file to follow along
  - Launch virtual machine
  - Open terminal window

```
$ cd ~/tutorial/aspect
$ gedit tutorial.prm &
```

- First section initializes the software
  - Lines starting by # provides comments

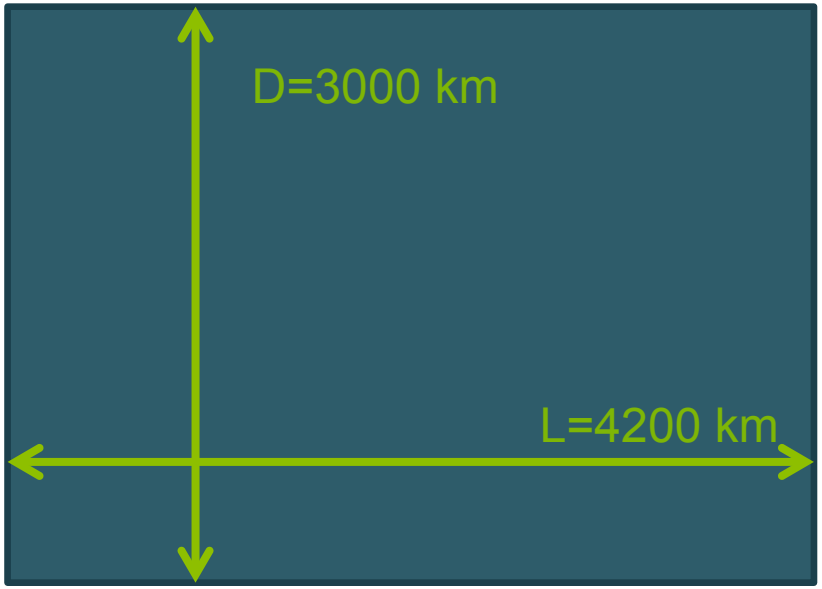
```
# At the top, we define the number of space dimensions we would like to
# work in:
set Dimension                                   = 2

# There are several global variables that have to do with what
# time system we want to work in and what the end time is. We
# also designate an output directory.
set Use years in output instead of seconds = true
set End time                                    = 5e10
set Output directory                            = output
```

Parameter file structure

- Subsections follow model design steps
- Fundamental equations for mantle convection are implied (details in model setting)
- Default Solution method
- Default values for many parameters

```
subsection Geometry model
subsection Mesh refinement
subsection Gravity model
subsection Material model
subsection Initial conditions
subsection Model settings
subsection Boundary temperature model
subsection Postprocess
```

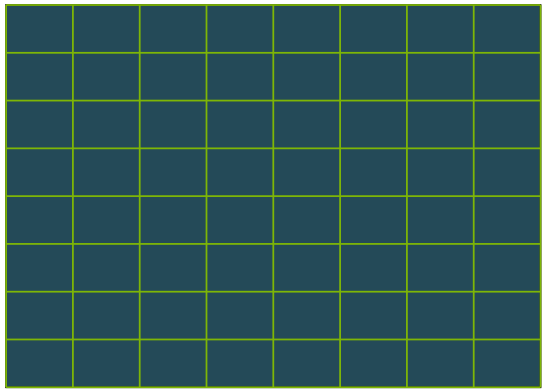
Model geometry



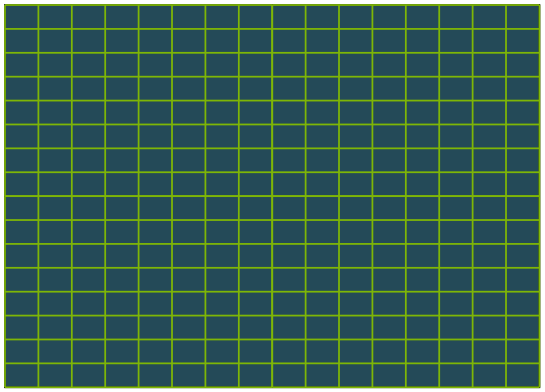

```
subsection Geometry model
  set Model name = box
  subsection Box
    set X extent = 4.2e6
    set Y extent = 3e6
  end
end
```

- Other options include “shell”
- Note the default unit: m

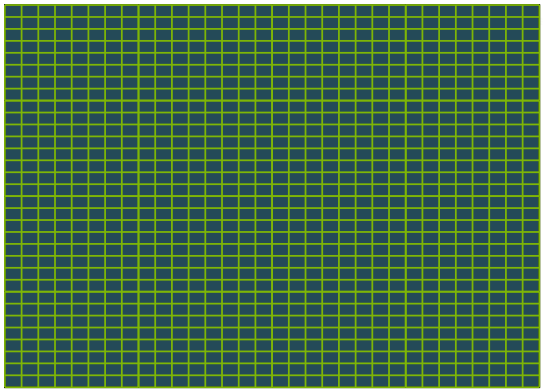
Discretization (mesh)



`Refine = 3` (8x8 cells)



`Refine = 4` (8x8 cells)



`Refine = 5` (32x32 cells)

- Initial global refinement controls "grid specig"
- Adaptive mesh refinement is turned off
- You will vary refinement to see what difference it makes.

```
subsection Mesh refinement
  set Initial global refinement                = 3
  set Initial adaptive refinement              = 0
  set Time steps between mesh refinement       = 0
end
```

Model parameters

- Other quantities have default values
  - k=4.7 W/m/K
  - C_p=1250 J/kg/K
  - ρ_0=3300 J/kg/K
  - $K=k/\rho_0 C_p=1.1394\times10^{-6}$ m^2/s
  - $\alpha=2\times10^{-5}$ K^{-1}

```
subsection Gravity model
  set Model name = vertical
  subsection Vertical
    set Magnitude = 9.81
  end
end

subsection Material model
  set Model name = simple
  subsection Simple model
    set Viscosity                    = 5.10452E24
  end
end
```

- What matters is the Rayleigh number

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

- Change viscosity to adjust Ra

$$\eta = \frac{\rho_0 g \alpha \Delta T D^3}{\mathrm{Ra}\,\kappa} = \frac{5.10542\times10^{28}}{\mathrm{Ra}}$$

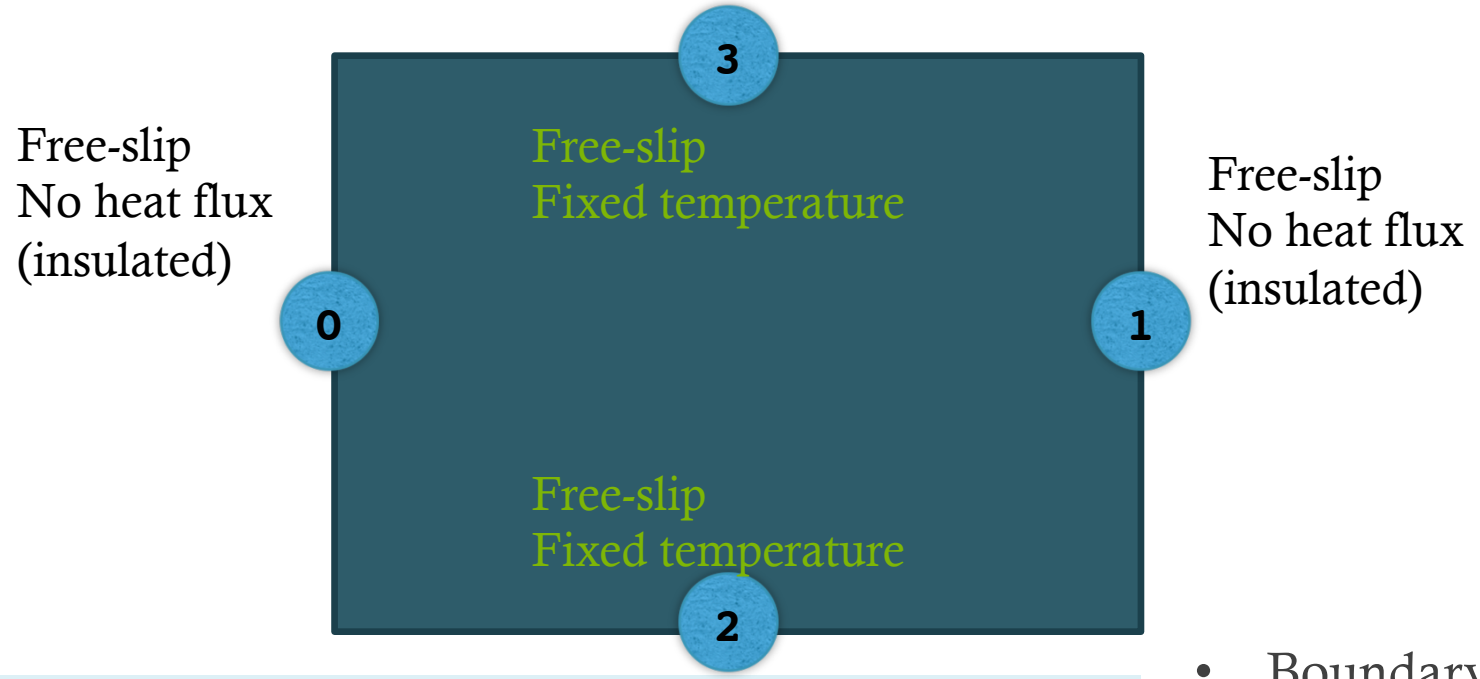
Setup initial conditions

- Linear temperature gradient from top to bottom, with sinusoidal perturbation of amplitude p and wavelength k
- Helps the development of convective instability
- Upwelling favored on left of the model

$$T = T_{\text{top}} + \left(T_{\text{bottom}} - T_{\text{top}}\right)\left[1 - \frac{y}{D} - p\cos\left(\frac{k\pi x}{L}\right)\sin\left(\frac{k\pi y}{D}\right)\right]$$

```
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
```

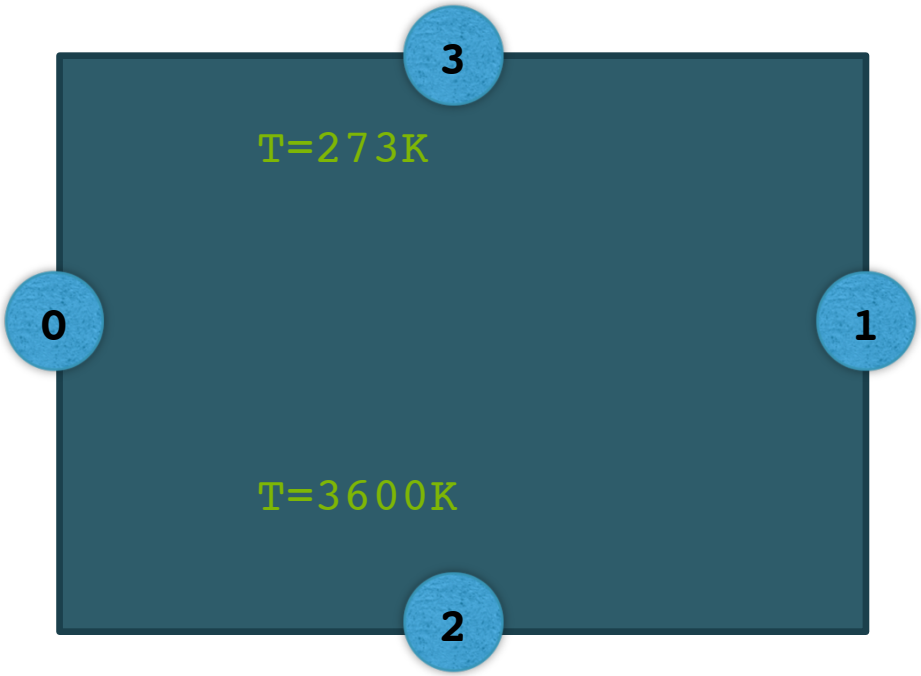
Prepare for boundary conditions




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

- Boundary numbering convention associated with geometrical object

Assign boundary conditions




```
subsection Boundary temperature model
  set Model name = box
  subsection Box
    set Bottom temperature = 3600
    set Top temperature    = 273
  end
end
```

- `Boundary temperature model /Box` assigns `Bottom Temperature` to the boundary with minimal z-value and `Top Temperature` to the boundary with maximum z-value
- Details in the aspect documentation

Postprocessing

- Setup basic analysis and fields to be stored on the computer

```
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 = vtu
  end
  subsection Tracers
    set Number of tracers = 1000
    set Time between data output = 1e7
    set Data output format = vtu
  end
end
```

Run ASPECT

- Open a terminal window
- Change to the appropriate directory

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

- Run ASPECT with the tutorial parameter file and log the output to a file named progress.txt (this should take about 20 seconds)

```
$ ./aspect tutorial.prm > progress.txt
```

- Open the log

```
$ gedit output/progress.txt
```

- Check the Rayleigh number!

Log file: initial state

```
-----------------------------------------------------------------------------
-- This is ASPECT, the Advanced Solver for Problems in Earth's ConvecTion.
--     . version 1.1
--     . running in OPTIMIZED mode
--     . running with 1 MPI process
--     . using Trilinos
-----------------------------------------------------------------------------

Number of active cells: 64 (on 4 levels)
Number of degrees of freedom: 948 (578+81+289)

*** Timestep 0:  t=0 years
   Solving temperature system... 0 iterations.
   Rebuilding Stokes preconditioner...
   Solving Stokes system... 7 iterations.

   Postprocessing:

     Reference density (kg/m^3):                    3300
     Reference gravity (m/s^2):                     9.81
     Reference thermal expansion (1/K):             2e-05
     Temperature contrast across model domain (K): 3327
     Model domain depth (m):                        3e+06
     Reference thermal diffusivity (m^2/s):         1.13939e-06
     Reference viscosity (Pas):                     5.10452e+24
     Ra number:                                     10000
     k_value:                                       4.7
     reference_cp:                                  1250
     reference_thermal_diffusivity:                 1.13939e-06

     RMS, max velocity:                  2.34e-05 m/year, 3.79e-05 m/year
     Temperature min/avg/max:            273 K, 1936 K, 3600 K
     Heat fluxes through boundary parts: -0.42 W, 0.42 W, -2.189e+04 W, 2.189e+04 W
     Writing graphical output:           output/solution-00000
     Advecting particles:                done. Writing particle graphical output output/particle-00000
```

Check Rayleigh number!

Initial heat flux?

Log file: Time stepping

```
*** Timestep 1:  t=4.93077e+09 years
   Solving temperature system... 23 iterations.
   Solving Stokes system... 13 iterations.

   Postprocessing:
     RMS, max velocity:                  9.72e-05 m/year, 0.000158 m/year
     Temperature min/avg/max:            273 K, 1936 K, 3600 K
     Heat fluxes through boundary parts: -1.541 W, 1.612 W, -2.211e+04 W, 2.211e+04 W
     Writing graphical output:           output/solution-00001
     Advecting particles:                done. Writing particle graphical output output/particle-00001

*** Timestep 2:  t=6.11497e+09 years
   Solving temperature system... 14 iterations.
   Solving Stokes system... 14 iterations.

   Postprocessing:
     RMS, max velocity:                  0.000189 m/year, 0.000308 m/year
     Temperature min/avg/max:            273 K, 1936 K, 3600 K
     Heat fluxes through boundary parts: -3.605 W, 3.599 W, -2.28e+04 W, 2.281e+04 W
     Writing graphical output:           output/solution-00002
     Advecting particles:                done. Writing particle graphical output output/particle-00002 ...

Etc.
```

Log file: Termination

```
*** Timestep 231:  t=5e+10 years
   Solving temperature system... 5 iterations.
   Solving Stokes system... 5 iterations.

   Postprocessing:
     RMS, max velocity:                   0.000635 m/year, 0.00097 m/year
     Temperature min/avg/max:             273 K, 1936 K, 3600 K
     Heat fluxes through boundary parts: -2168 W, 2276 W, -9.541e+04 W, 9.584e+04 W
     Writing graphical output:            output/solution-00231
     Advecting particles:                 done. Writing particle graphical output output/particle-00231

Termination requested by criterion: end time


+---------------------------------------------+------------+------------+
| Total wallclock time elapsed since start    |      12.6s |            |
|                                             |            |            |
| Section                          | no. calls |  wall time | % of total |
+----------------------------------+-----------+------------+------------+
| Assemble Stokes system           |       232 |      0.17s |       1.3% |
| Assemble temperature system      |       232 |      1.08s |       8.6% |
| Build Stokes preconditioner      |         1 |    0.0218s |      0.17% |
| Build temperature preconditioner|       232 |     0.175s |       1.4% |
| Solve Stokes system              |       232 |       0.8s |       6.4% |
| Solve temperature system         |       232 |     0.133s |       1.1% |
| Initialization                   |         2 |    0.0832s |      0.66% |
| Postprocessing                   |       232 |      9.75s |        77% |
| Setup dof systems                |         1 |    0.0883s |       0.7% |
+----------------------------------+-----------+------------+------------+
```

Final heat flux?

Nusselt Number?

$$\mathrm{Nu} = \frac{Q/L}{k\,\Delta T/D}$$

Initial convection calculation

- Rayleigh number 10,000

$$\mathrm{Ra} = \frac{\rho_0 g \alpha \Delta T D^3}{\eta \kappa} = \frac{3300 * 9.81 * 2 \times 10^{-5} * 3327 * \left(3 \times 10^6\right)^3}{5.10452 \times 10^{24} * 1.1394 \times 10^{-6}}$$

- Diffusive heat flux

$$k \frac{\Delta T}{D} = 4.7 * \frac{3327}{3 \times 10^3} = 5.2123 \times 10^{-3}\ \mathrm{W/m^2}$$

- Initial heat flux (boundary 3) Q/L:

$$q = \frac{Q}{L} = \frac{2.211 \times 10^4}{4.2 \times 10^6} = 5.2643 \times 10^3\ \mathrm{W/m^2}$$

- Final Nu:

$$Nu = \frac{Q/L}{k \Delta T / D} = \frac{9.584 \times 10^4 / 4.2 \times 10^6}{5.2123 \times 10^{-3}} = 4.38$$

Model history

- Check "statistics" output file

  `$ gedit output/statistics &`

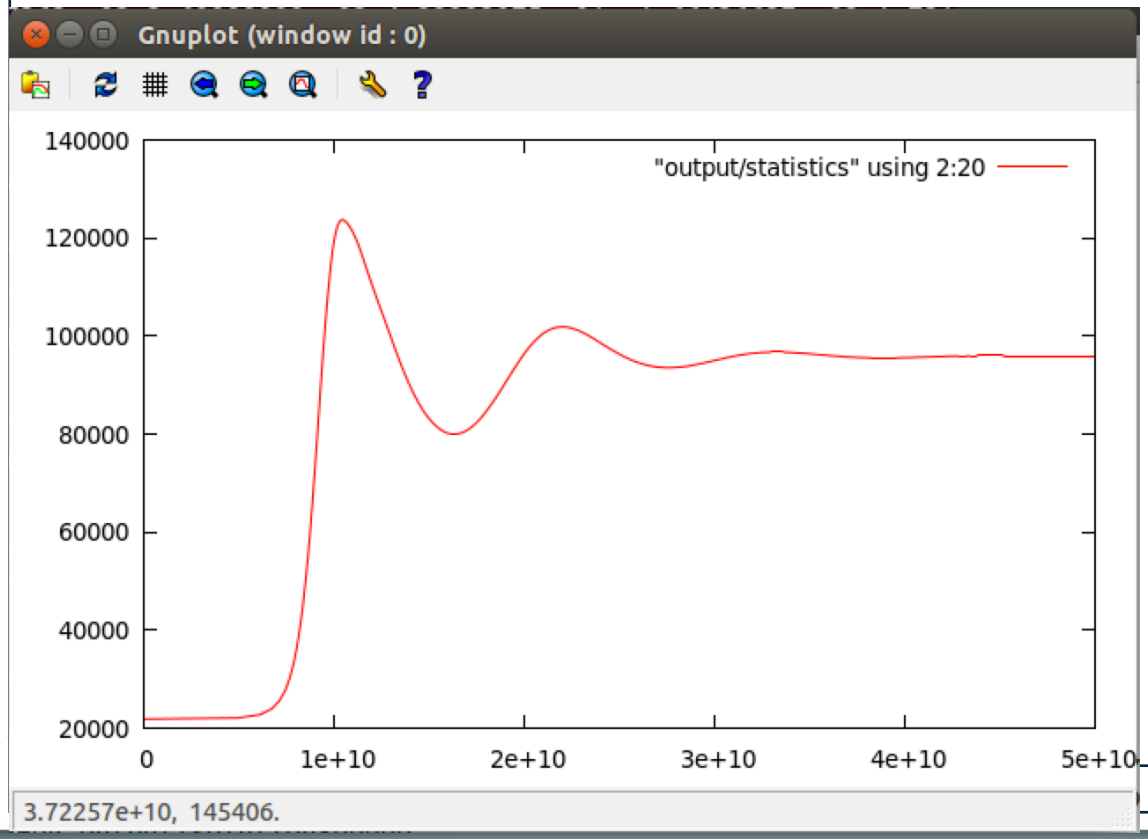
  - Files includes a table of statistics and diagnostic information

```
# 1: Time step number
# 2: Time (years)
# 3: Number of mesh cells
# 4: Number of Stokes degrees of freedom
# 5: Number of temperature degrees of freedom
# 6: Iterations for temperature solver
# 7: Iterations for Stokes solver
# 8: Velocity iterations in Stokes preconditioner
# 9: Schur complement iterations in Stokes preconditioner
# 10: Time step size (years)
# 11: RMS velocity (m/year)
# 12: Max. velocity (m/year)
# 13: Minimal temperature (K)
# 14: Average temperature (K)
# 15: Maximal temperature (K)
# 16: Average nondimensional temperature (K)
# 17: Outward heat flux through boundary with indicator 0 (W)
# 18: Outward heat flux through boundary with indicator 1 (W)
# 19: Outward heat flux through boundary with indicator 2 (W)
# 20: Outward heat flux through boundary with indicator 3 (W)
# 21: Visualization file name
  0 0.0000e+00 64 659 289  0  7  8  7 4.9308e+09 2.33665793e-05
3.79495935e-05 2.73000000e+02 1.93650000e+03 3.60000000e+03
5.00000000e-01 -4.20043660e-01 4.20043660e-01 -2.18916600e+04
2.18916600e+04 output/solution-00000
  1 4.9308e+09 64 659 289 23 13 14 14 1.1842e+09 9.72361537e-05
1.58042252e-04 2.73000000e+02 1.93646647e+03 3.60000000e+03
4.99989922e-01 -1.54068209e+00 1.61246895e+00 -2.21096633e+04
2.21108422e+04 output/solution-00001
```

Plotting model history

- Quick plot using gnuplot. Use the command line

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

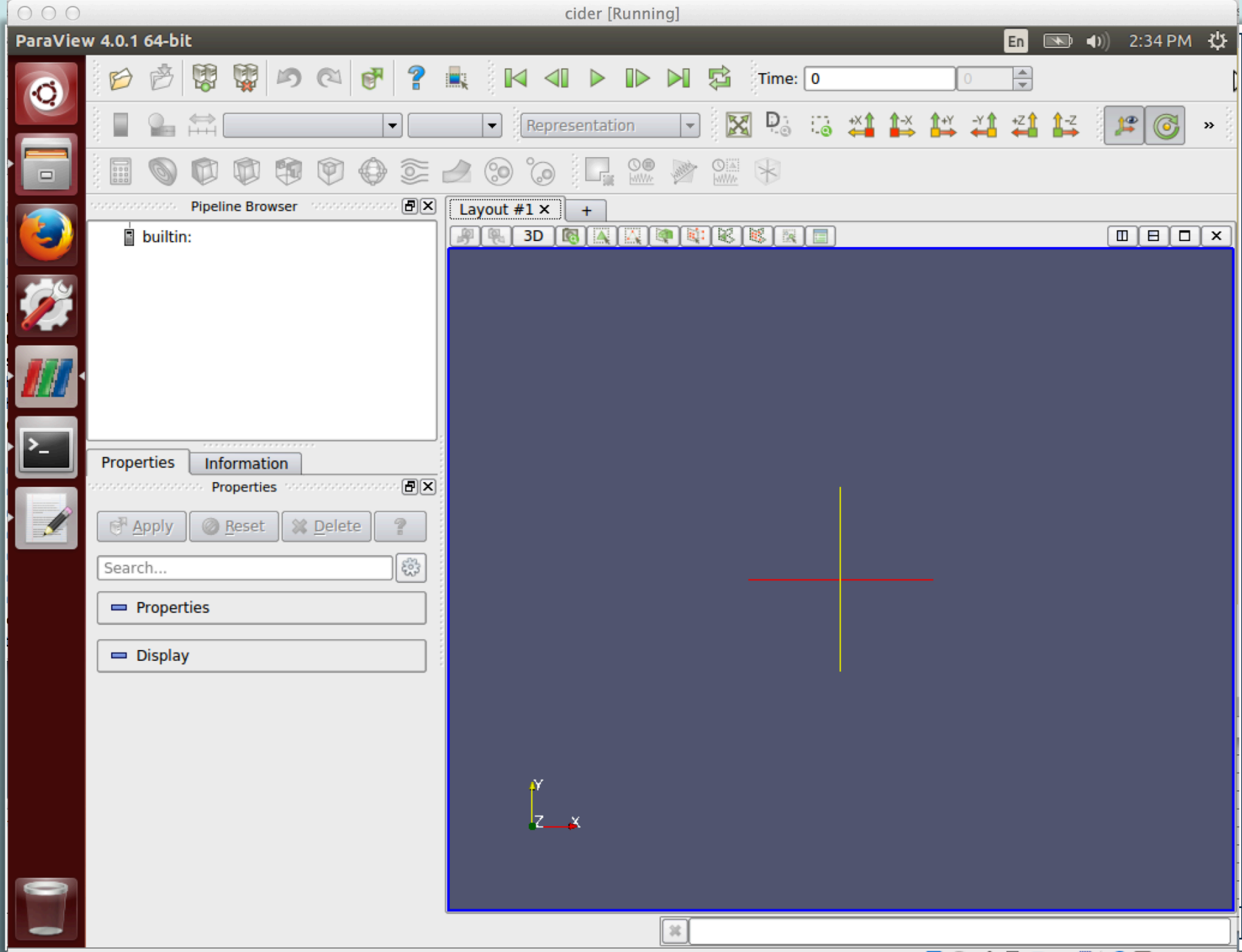


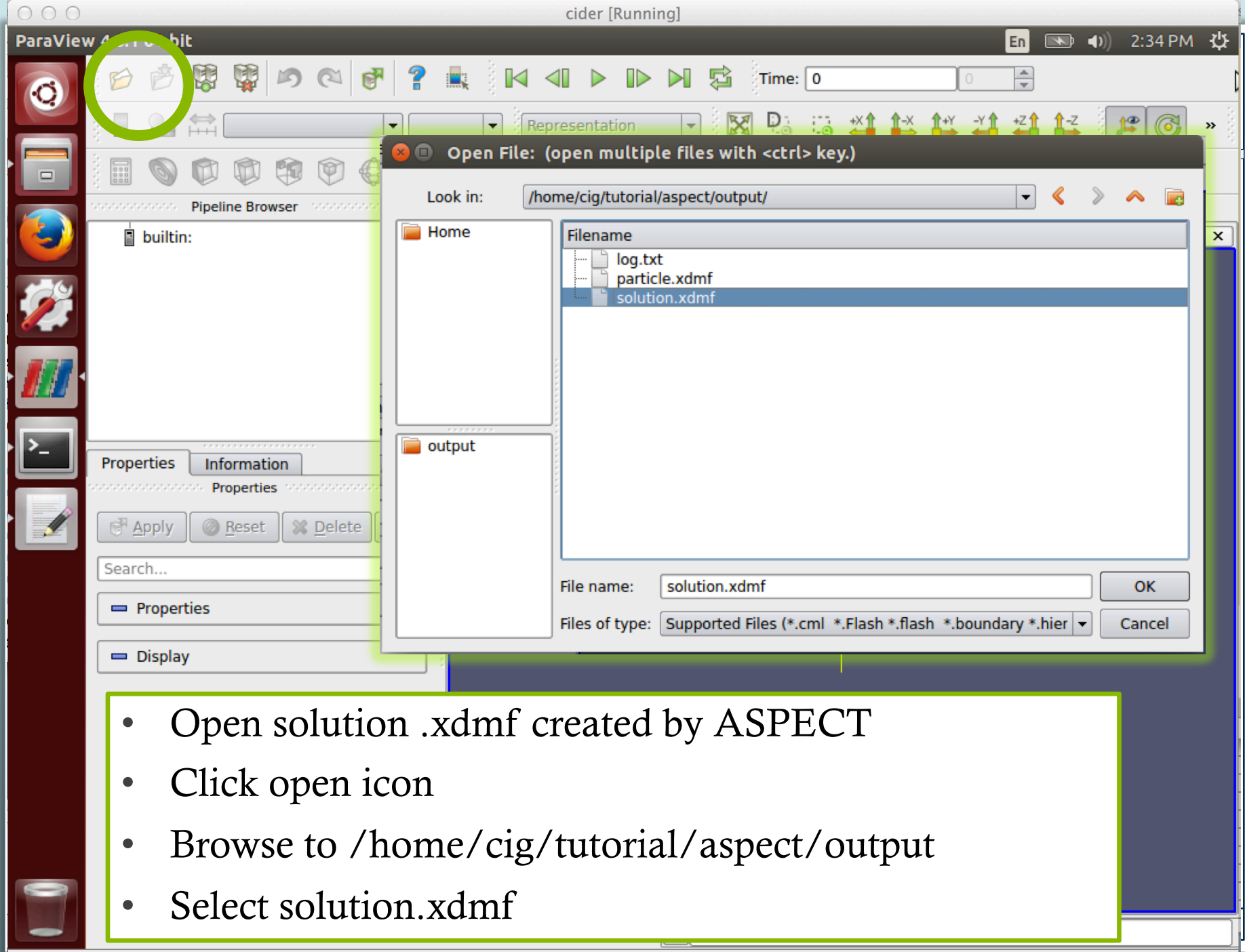
How does the surface heat flux change over time?

Is this evolution compatible with the information from the log?

Visualization with ParaView

- Open ParaView on the virtual machine
  - Program designed for the visualization of large datasets
  - Works in parallel
  - Support fields and particle clouds in 3D
  - Visualization tools include isosurfaces (contours), slices, streamlines, volume rendering, and other complex techniques

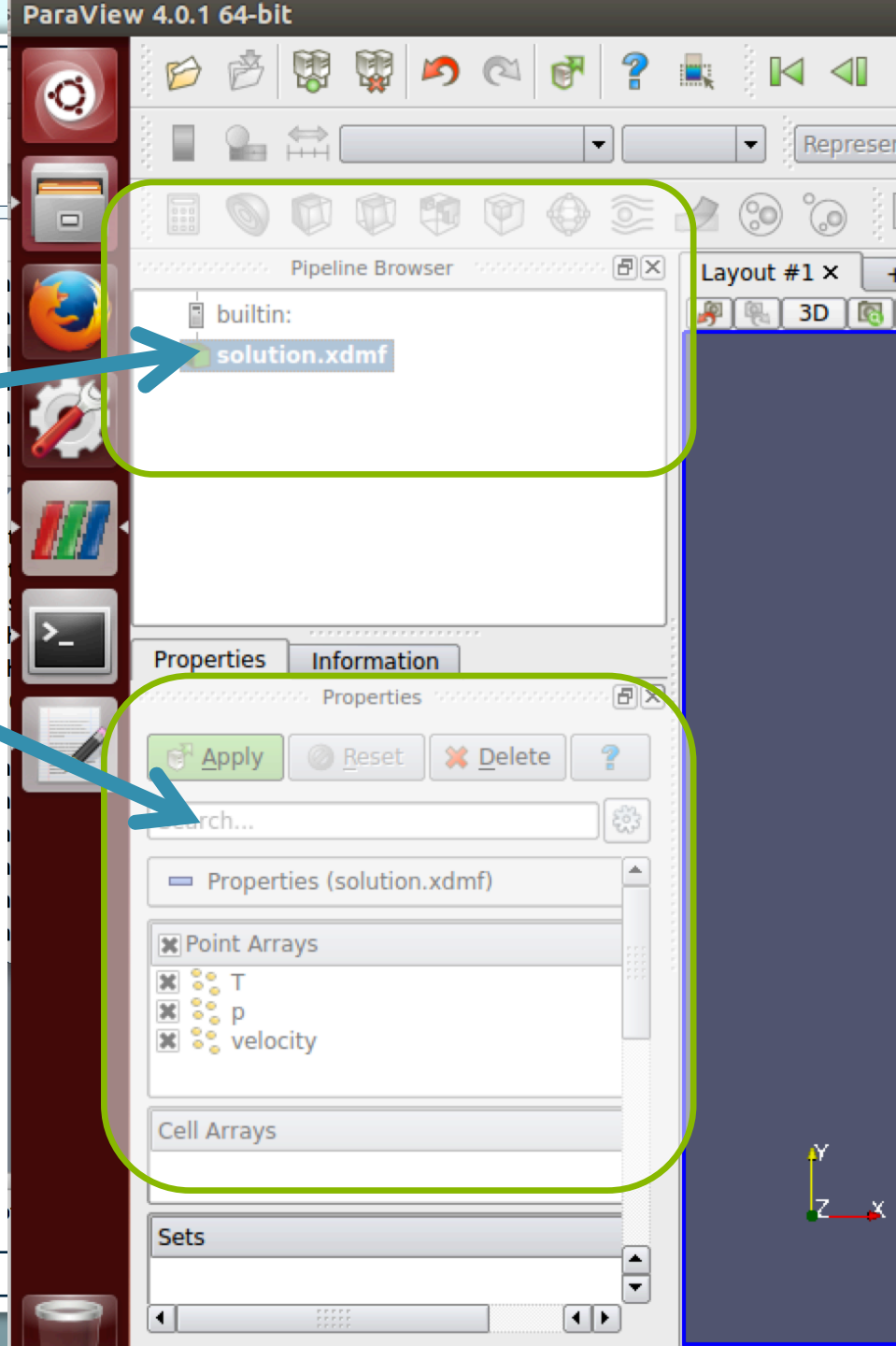

cider [Running]
ParaView 4.0.1 64-bit
En
2:34 PM
Time:
0
Representation
Pipeline Browser
builtin:
Layout #1
3D
Properties
Information
Properties
Apply
Reset
Delete
Search...
Properties
Display
Y
Z
X
Left ⌘



- Open solution .xdmf created by ASPECT
- Click open icon
- Browse to /home/cig/tutorial/aspect/output
- Select solution.xdmf

Visualizing Fields

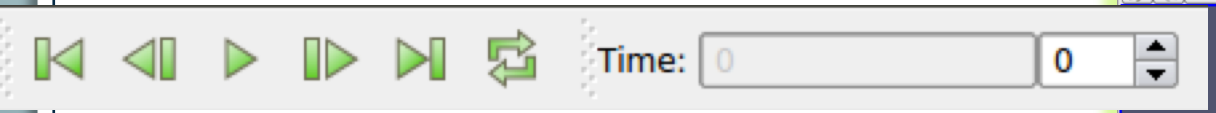
- The file appears the Pipeline Browser
- Check the properties (variables) in the object inspector
- Click “Apply” to show the field in the view area
  - Default shows temperature



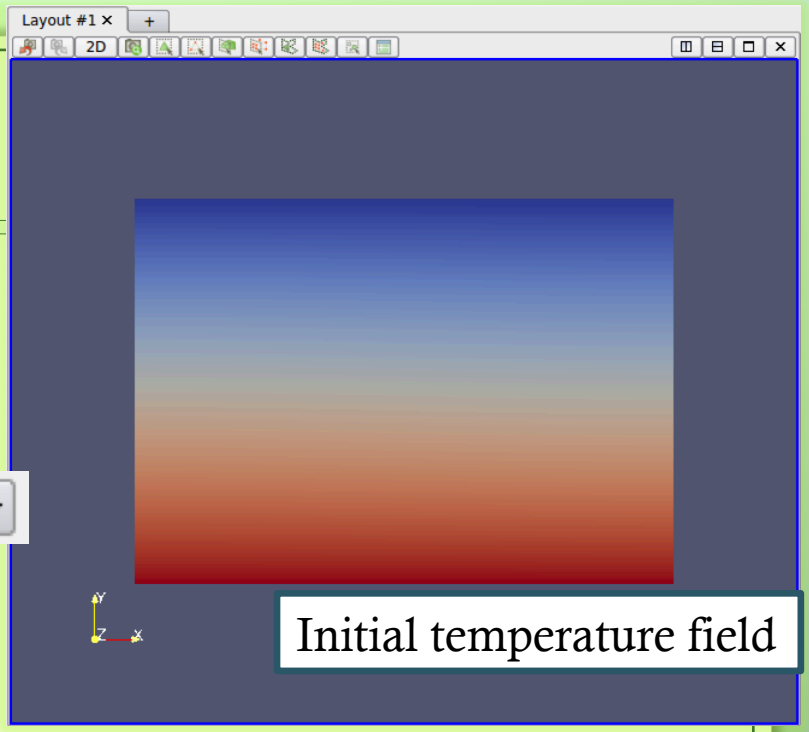
Temperature

- Default visualization is temperature field

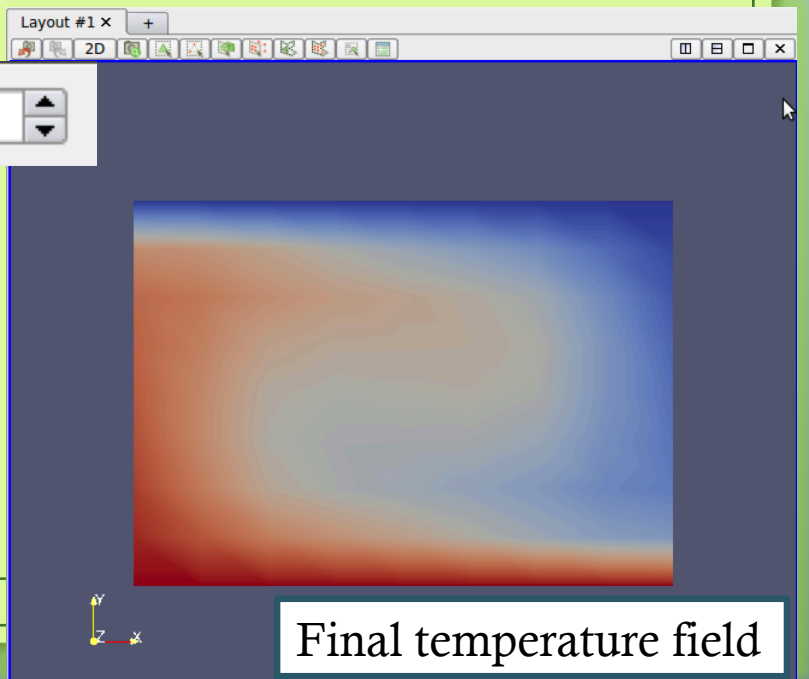
- Use the toolbar to watch how the temperature changes



- Near the end, is the temperature field static? Is the velocity field static? Is the material moving?



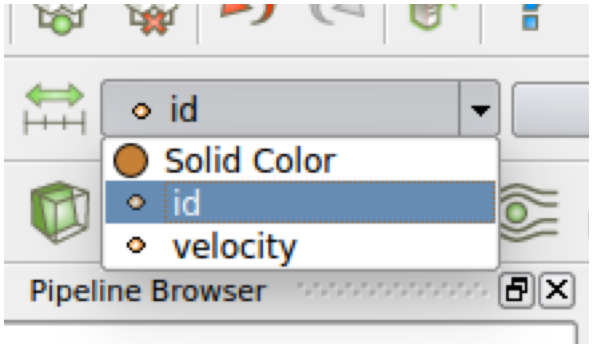
Initial temperature field

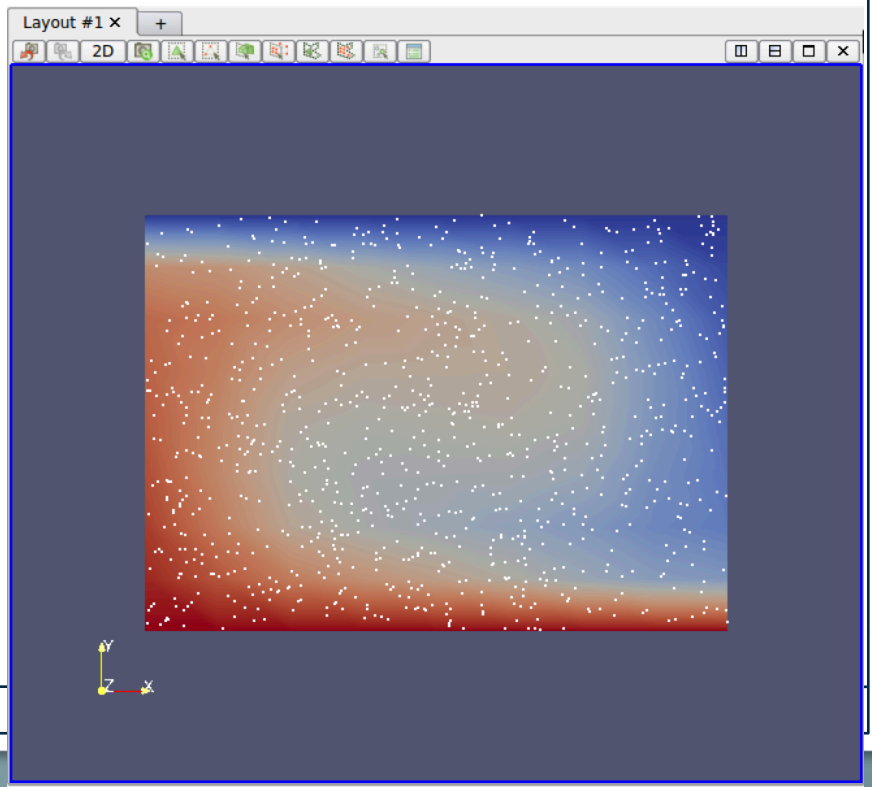


Final temperature field

Visualizing particles

- Open the file particle.xdmf and click “Apply”
  - By default, particles are colored by ID. Change the coloring scheme to “Solid Color” to make them all white.
- So, are the particles static at the end of the simulation?
- Describe the flow field. Where is the upwelling? Where is the downwelling?





Nusselt-Rayleigh relation

- Split the class into groups
- Copy (use `cp` command), Rename (use `cp` command)and modify `tutorial.prm`
  - Change end-time, mesh refinement, Rayleigh number (viscosity)
  - (optional) change the output directory
- Run the simulation
  - To save time run in the background, pushing the output to a file

```
> ./aspect Ra1e5R4.prn > LogRa1e5R4.txt &
```

- Visualize the results
- Report the Nusselt number

$$\mathrm{Nu} = \frac{Q/L}{k\,\Delta T/D} = \frac{Q/4.2\times10^{6}}{4.7*(3600-273)/3\times10^{6}} = \frac{Q}{21892}$$

- In theory, there is a power-law relation between Ra and Nu

Nusselt-Rayleigh relationship

	Ra=4,000	Ra=20,000	Ra=100,000	Ra=500,000
End time	2×10^{11}	5×10^{10}	3×10^{10}	1×10^{10}
Viscosity	1.275×10^{25}	2.5522×10^{24}	5.1045×10^{24}	1.0209×10^{10}
Q (refine =3)				
Q (refine =4)				
Q (refine =5)				
Nu (refine =3)				
Nu (refine =4)				
Nu (refine =5)				

- Plot Nu vs Ra
- Do you have a power law relation? Is for, what is the power law exponent?