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
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 stratification
- Conductive heat flux

\[ q = k \frac{\Delta T}{D} \]

<table>
<thead>
<tr>
<th>q</th>
<th>k</th>
<th>( \Delta T )</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat flux</td>
<td>Thermal conductivity</td>
<td>Temperature change</td>
<td>Thickness</td>
</tr>
</tbody>
</table>
Convection intensifies heat flux

Cooling plate (heat loss)

Heating plate (heat input)

Well-mixed isotherm interior

Temperature

cold

hot
Nusselt what?

- Hot, low density material wants to rise.
- If viscosity is low enough: convection!
- Hot material near the surface generates high heat flux (boundary layer)

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

\[ Nu = \frac{q}{k \Delta T/D} \]

<table>
<thead>
<tr>
<th>( \rho_0 )</th>
<th>g</th>
<th>( \alpha )</th>
<th>( \Delta T )</th>
<th>D</th>
<th>( \eta )</th>
<th>( \kappa )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>gravity</td>
<td>Expansion coefficient</td>
<td>Temperature change</td>
<td>Thickness</td>
<td>viscosity</td>
<td>Thermal diffusivity</td>
</tr>
</tbody>
</table>
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
  \[
  \rho C_p \left( \frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) - \nabla \cdot (k \nabla T) = \rho H + \frac{\partial \rho}{\partial T} T \mathbf{v} \cdot \mathbf{g} + 2\eta \left[ \dot{\varepsilon} - \frac{1}{3} (\nabla \cdot \mathbf{v}) \mathbf{I} \right] : \left[ \dot{\varepsilon} - \frac{1}{3} (\nabla \cdot \mathbf{v}) \mathbf{I} \right]
  \]

<table>
<thead>
<tr>
<th>( \mathbf{v} )</th>
<th>Velocity</th>
<th>m/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>( P )</td>
<td>Pressure</td>
<td>Pa</td>
</tr>
<tr>
<td>( T )</td>
<td>Temperature</td>
<td>K</td>
</tr>
<tr>
<td>( \dot{\varepsilon} \equiv \frac{1}{2} (\nabla \mathbf{v} + \nabla \mathbf{v}^T) )</td>
<td>Strain rate</td>
<td>s(^{-1})</td>
</tr>
<tr>
<td>( \eta )</td>
<td>Viscosity</td>
<td>Pa s</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( \rho )</th>
<th>Density</th>
<th>Kg/m(^3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( g )</td>
<td>Gravity</td>
<td>m/s(^1)</td>
</tr>
<tr>
<td>( C_p )</td>
<td>Heat capacity</td>
<td>J/kg/K</td>
</tr>
<tr>
<td>( k )</td>
<td>Heat conductivity</td>
<td>W/m/K</td>
</tr>
<tr>
<td>( H )</td>
<td>Heat production</td>
<td>W/kg</td>
</tr>
</tbody>
</table>
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


• Open VirtualBox
• In the File menu, select Import Appliance
• Click on the yellow folder and browse to wherever you saved the [cider.ova](#) 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
• 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 succeeds, 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

```plaintext
# 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
Other options include “shell”

Note the default unit: m
Discretization (mesh)

- 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
  - \( k = 4.7 \text{ W/m/K} \)
  - \( C_p = 1250 \text{ J/kg/K} \)
  - \( \rho_0 = 3300 \text{ J/kg/K} \)
  - \( K = k / \rho_0 C_p = 1.1394 \times 10^{-6} \text{ m}^2/\text{s} \)
  - \( \alpha = 2 \times 10^{-5} \text{ K}^{-1} \)

- What matters is the Rayleigh number
  \[
  Ra = \frac{\rho_0 g \alpha \Delta T D^3}{\eta \kappa}
  \]

- Change viscosity to adjust \( Ra \)
  \[
  \eta = \frac{\rho_0 g \alpha \Delta T D^3}{Ra \kappa} = 5.10542 \times 10^{28}
  \]

```plaintext
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
```

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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

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

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_{\text{top}}=273, T_{\text{bottom}}=3600
    set Function expression = T_{\text{top}} + (T_{\text{bottom}}-T_{\text{top}}) \left[ 1 - \frac{y}{D} - p \cos\left(\frac{k\pi x}{L}\right) \sin\left(\frac{k\pi y}{D}\right) \right]
  end
end
Prepare for boundary conditions

- Boundary numbering convention associated with geometrical object

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

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Free-slip
No heat flux
(insulated)

Free-slip
Fixed temperature

Free-slip
Fixed temperature
Assign boundary conditions

- 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.

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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
```
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/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
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?

\[
\text{Nu} = \frac{Q}{L} \left(\frac{k \Delta T}{D}\right)
\]
Initial convection calculation

- Rayleigh number 10,000
  \[
  Ra = \frac{\rho_0 g \alpha \Delta T D^3}{\eta \kappa} = \frac{3300 \times 9.81 \times 2 \times 10^{-5} \times 3327 \times (3 \times 10^6)^3}{5.10452 \times 10^{24} \times 1.1394 \times 10^{-6}}
  \]
- Diffusive heat flux
  \[
  k \frac{\Delta T}{D} = 4.7 \times \frac{3327}{3 \times 10^3} = 5.2123 \times 10^{-3} \text{ W/m}^2
  \]
- Initial heat flux (boundary 3) Q/L:
  \[
  q = \frac{Q}{L} = \frac{2.211 \times 10^4}{4.2 \times 10^6} = 5.2643 \times 10^3 \text{ W/m}^2
  \]
- 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

<table>
<thead>
<tr>
<th>#</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Time step number</td>
</tr>
<tr>
<td>2</td>
<td>Time (years)</td>
</tr>
<tr>
<td>3</td>
<td>Number of mesh cells</td>
</tr>
<tr>
<td>4</td>
<td>Number of Stokes degrees of freedom</td>
</tr>
<tr>
<td>5</td>
<td>Number of temperature degrees of freedom</td>
</tr>
<tr>
<td>6</td>
<td>Iterations for temperature solver</td>
</tr>
<tr>
<td>7</td>
<td>Iterations for Stokes solver</td>
</tr>
<tr>
<td>8</td>
<td>Velocity iterations in Stokes preconditioner</td>
</tr>
<tr>
<td>9</td>
<td>Schur complement iterations in Stokes preconditioner</td>
</tr>
<tr>
<td>10</td>
<td>Time step size (years)</td>
</tr>
<tr>
<td>11</td>
<td>RMS velocity (m/year)</td>
</tr>
<tr>
<td>12</td>
<td>Max. velocity (m/year)</td>
</tr>
<tr>
<td>13</td>
<td>Minimal temperature (K)</td>
</tr>
<tr>
<td>14</td>
<td>Average temperature (K)</td>
</tr>
<tr>
<td>15</td>
<td>Maximal temperature (K)</td>
</tr>
<tr>
<td>16</td>
<td>Average nondimensional temperature (K)</td>
</tr>
<tr>
<td>17</td>
<td>Outward heat flux through boundary with indicator 0 (W)</td>
</tr>
<tr>
<td>18</td>
<td>Outward heat flux through boundary with indicator 1 (W)</td>
</tr>
<tr>
<td>19</td>
<td>Outward heat flux through boundary with indicator 2 (W)</td>
</tr>
<tr>
<td>20</td>
<td>Outward heat flux through boundary with indicator 3 (W)</td>
</tr>
<tr>
<td>21</td>
<td>Visualization file name</td>
</tr>
</tbody>
</table>

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 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 2.61108422e+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

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

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

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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?
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

\[
\begin{align*}
\text{Nu} &= \frac{Q/L}{k \Delta T/D} = \frac{Q/4.2 \times 10^6}{4.7 \times (3600 - 273)/3 \times 10^6} = \frac{Q}{21892}
\end{align*}
\]
- In theory, there is a power-law relation between Ra and Nu
### Nusselt-Rayleigh relationship

<table>
<thead>
<tr>
<th></th>
<th>Ra=4,000</th>
<th>Ra=20,000</th>
<th>Ra=100,000</th>
<th>Ra=500,000</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>End time</strong></td>
<td>$2 \times 10^{11}$</td>
<td>$5 \times 10^{10}$</td>
<td>$3 \times 10^{10}$</td>
<td>$1 \times 10^{10}$</td>
</tr>
<tr>
<td><strong>Viscosity</strong></td>
<td>$1.275 \times 10^{25}$</td>
<td>$2.5522 \times 10^{24}$</td>
<td>$5.1045 \times 10^{24}$</td>
<td>$1.0209 \times 10^{10}$</td>
</tr>
<tr>
<td>Q (refine =3)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Q (refine =4)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Q (refine =5)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nu (refine =3)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nu (refine =4)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nu (refine =5)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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