ASPECT tutorial
Part II: Melt transport

Juliane Dannberg,
Rene Gassmöller, John Naliboff
Starting the model...

• This will take a while...
• Start by going to the Desktop directory:
  `cd Desktop`
Starting the model...

- Then start the model by typing:
  
  mpirun -np 2 aspect
  ../aspect/cookbooks/mid_ocean_ridge.prm
Starting the model...

• This should give you output like this
• We will let this model run and come back later
Outline

1. Theory
2. Methods
3. Example
4. Playtime

Mid-ocean ridges

From http://www.phschool.com
The problem

\[ \rho \quad \text{density} \quad \eta^* \quad \text{shear viscosity} \quad \xi^* \quad \text{compaction viscosity} \quad K_D \quad \text{Darcy coefficient} \]

Partially molten

Darcy coefficient \( K_D \sim \phi^3 \)

Shear, compaction viscosity \( \eta, \xi = \eta(\phi), \xi(\phi) \)
Excellent introduction:

Very comprehensive lecture notes:
http://foalab.earth.ox.ac.uk/files/IntroMagmaLectures.pdf
Equations: Mantle convection

Mass conservation

\[ \nabla \cdot (\rho \mathbf{u}) = 0 \]

Momentum conservation

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

Energy conservation

\[ \rho C_p \left( \frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) - \nabla \cdot k \nabla T = \ldots \text{ (source terms)} \]

u_s, solid velocity
p, pressure
\rho, density
g, gravity
Equations: Magma/mantle dynamics

Mass conservation

\[ \frac{\partial}{\partial t} [\rho_f \phi] + \nabla \cdot [\rho_f \phi \mathbf{u}_f] = \Gamma \]

\[ \frac{\partial}{\partial t} [\rho_s (1 - \phi)] + \nabla \cdot [\rho_s (1 - \phi) \mathbf{u}_s] = -\Gamma \]

Momentum conservation

\[ \phi (\mathbf{u}_f - \mathbf{u}_s) = -K_D (\nabla p_f - \rho_f \mathbf{g}) \]

\[ -\nabla \cdot \left[ 2\eta^* \left( \varepsilon(\mathbf{u}_s) - \frac{1}{3} (\nabla \cdot \mathbf{u}_s) \mathbf{1} \right) + \xi^*(\nabla \cdot \mathbf{u}_s) \mathbf{1} \right] + \nabla p_f = \bar{\rho} \mathbf{g} \]

Melt advection

\[ \frac{\partial \phi}{\partial t} + \mathbf{u}_s \cdot \nabla \phi = \frac{\Gamma}{\rho_s} + (1 - \phi) (\nabla \cdot \mathbf{u}_s + \kappa_s \rho_s \mathbf{g} \cdot \mathbf{u}_s) \]

Energy conservation

\[ \rho C_p \left( \frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) - \nabla \cdot k \nabla T = \ldots \text{ (source terms)} \]

\( u_{s,f} \): solid, fluid velocity
\( \phi \): porosity
\( p_f \): fluid pressure
\( p_c \): compaction pressure
\( \rho_{s,f} \): density
\( \mathbf{g} \): gravity
\( \Gamma \): melting rate
Equations: Magma/mantle dynamics

Mass conservation

\[
\frac{\partial}{\partial t} [\rho_f \phi] + \nabla \cdot [\rho_f \phi \mathbf{u}_f] = \Gamma \\
\frac{\partial}{\partial t} [\rho_s (1 - \phi)] + \nabla \cdot [\rho_s (1 - \phi) \mathbf{u}_s] = -\Gamma
\]

Solid and fluid mass are conserved.

The difference between solid and melt velocity depends on the permeability and pressure gradients in the melt.

Momentum conservation

\[
\phi (\mathbf{u}_f - \mathbf{u}_s) = -K_D (\nabla p_f - \rho_f g)
\]

\[-\nabla \cdot \left[ 2\eta^* \left( \varepsilon(\mathbf{u}_s) - \frac{1}{3} (\nabla \cdot \mathbf{u}_s) \mathbf{1} \right) + \xi^* (\nabla \cdot \mathbf{u}_s) \mathbf{1} \right] + \nabla p_f = \bar{\rho} g
\]

In addition to being sheared... the solid can also compact and dilate as melt flows in and out.
Scaling

• Compaction length

\[ \delta = \sqrt{\frac{(\xi + 4\eta/3)k}{\eta_f}} \]

Describes the intrinsic length scale of melt transport: length scale over which the compaction pressure responds to variations in fluid flux

• Separation flux:

\[ \phi w = \frac{k\Delta \rho g}{\eta_f} \]

is an estimate of the (gravity drive) melt flux relative to the solid
Shear bands

Magmatic shear bands
Solitary waves
Methods
PDE system

Eliminating $u_f$ and introducing the compaction pressure $p_c$ leads to:

$$- \nabla \cdot \left[ 2\eta \left( \ddot{u}_s - \frac{1}{3} (\nabla \cdot u_s) 1 \right) \right] + \nabla p_f + \nabla p_c = \bar{\rho} \mathbf{g},$$

$$\nabla \cdot u_s - \nabla \cdot K_D \nabla p_f - K_D \nabla p_f \cdot \frac{\nabla \rho_f}{\rho_f} = -\nabla \cdot (K_D \rho_f \mathbf{g})$$

$$+ \Gamma \left( \frac{1}{\rho_f} - \frac{1}{\rho_s} \right)$$

$$- \frac{\phi}{\rho_f} u_s \cdot \nabla \rho_f - (u_s \cdot \mathbf{g})(1 - \phi) \kappa_s \rho_s$$

$$- K_D \mathbf{g} \cdot \nabla \rho_f,$$

$$\nabla \cdot u_s + \frac{p_c}{\xi} = 0.$$
PDE system

\[-\nabla \cdot \left[ 2\eta \left( \dot{\varepsilon}(u_s) - \frac{1}{3}(\nabla \cdot u_s)\mathbf{1} \right) \right] + \nabla p_f + \nabla p_c = \bar{\rho} g,\]

\[\nabla \cdot u_s - \nabla \cdot K_D \nabla p_f - K_D \nabla p_f \cdot \frac{\nabla \rho_f}{\rho_f} = -\nabla \cdot (K_D \rho_f g)\]

\[\quad + \Gamma \left( \frac{1}{\rho_f} - \frac{1}{\rho_s} \right)\]

\[\quad - \frac{\phi}{\rho_f} u_s \cdot \nabla \rho_f - (u_s \cdot \mathbf{g})(1 - \phi)\kappa_s \rho_s\]

\[\quad - K_D g \cdot \nabla \rho_f,\]

\[\nabla \cdot u_s + \frac{p_c}{\xi} = 0.\]

Discretization yields the linear system

\[
\begin{pmatrix}
A & B^T & B^T \\
B & N & 0 \\
B & 0 & K
\end{pmatrix}
\begin{pmatrix}
U_s \\
P_f \\
P_c
\end{pmatrix} =
\begin{pmatrix}
F \\
G \\
0
\end{pmatrix}
\]
New formulation

From R. Grove, PhD thesis

\[
\begin{pmatrix}
A & B^T & B^T \\
B & N & 0 \\
B & 0 & K
\end{pmatrix}
\begin{pmatrix}
U_s \\
P_f \\
P_c
\end{pmatrix}
= 
\begin{pmatrix}
F \\
G \\
0
\end{pmatrix}
\]

- linearly dependent for \( \phi \to 0 \)
- \( K_D \to 0 \) for \( \phi \to 0 \)
  \((K_D \propto \phi^n, n = 2 \text{ or } 3)\)
- Last equation vanishes for \( \phi \to 0 \)
- \( P_c \to 0 \) for \( \phi \to 0 \)

From R. Grove, PhD thesis
New formulation: $\phi \to 0$

\[
\begin{pmatrix}
A & B^T & B^T \\
B & N & 0 \\
B & 0 & K
\end{pmatrix}
\begin{pmatrix}
U_s \\
P_f \\
P_c
\end{pmatrix}
= 
\begin{pmatrix}
F \\
G \\
0
\end{pmatrix}
\]

- Stokes system

- Linearly dependent for $\phi \to 0$

- $K_D \to 0$ for $\phi \to 0$  
  ($K_D \propto \phi^n, n = 2 \text{ or } 3$)

- Last equation vanishes for $\phi \to 0$

- Do not solve last equation if $\phi < \phi_{\text{min}}$
Constraints

1. Reformulate equations
2. Only solve the two-phase flow equations if the porosity is above a given limit, otherwise solve Stokes flow with one phase
   - Advantage: faster solver + recovery of Stokes solution for $\phi \to 0$
Mantle melting can be described as “reaction” between the solid and the fluid phase.

Thermodynamics: assumption of equilibrium (very fast reactions)

Geodynamics: reaction rates $q$

$$\frac{\partial c(t)}{\partial t} + u \cdot \nabla c(t) = q(c(t)),$$

where $c$ is a vector of compositions or phases.

Problems with accuracy/convergence of the non-linear solver, in particular if there is a threshold for melt transport.
Reactions: Operator Splitting

Solution: operator split, allows for different time steps

Instead of solving

$$\frac{\partial c(t)}{\partial t} + \mathbf{u} \cdot \nabla c(t) = q(c(t)),$$

we first solve the advection equation without reactions

$$\frac{\partial c(t)}{\partial t} + \mathbf{u} \cdot \nabla c(t) = 0$$

obtaining $\Delta c_A(t^{n+1})$ from $c(t^n)$,

and then resolve the reactions as a series of coupled ODEs, potentially with a different time step:

$$\frac{\partial c(t)}{\partial t} = q(c(t^n) + \Delta c_A(t^{n+1}))$$

obtaining $\Delta c_R(t^{n+1})$ from $c(t^n) + \Delta c_A(t^{n+1})$.

Allows for equilibrium & disequilibrium melting
Adaptive mesh refinement

Refine the mesh where melt is present
Model setup
Ingredients of a Model

Motivation: What is the question we want to answer?
- Equations ✔
- Geometry: Which region is part of the model?
- Mesh
- Material properties
  - How does the material deform?
  - What is the density?
- Initial conditions
- Boundary conditions: Can material/energy flow in and out?
- Solvers
- Postprocessing
Using the ASPECT GUI...

- We will look at the input file in the ASPECT-GUI:
  
  `aspect-gui
  ../../aspect/cookbooks/mid_ocean_ridge.prm`
Equations

Coupled Stokes/Darcy flow

Melting and freezing reactions + latent heat

Advection + Diffusion of heat

Stokes flow
<table>
<thead>
<tr>
<th>(Sub)Sections/Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nonlinear solver scheme</td>
<td>iterated Advection and Stokes</td>
</tr>
<tr>
<td>Adiabatic surface temperature</td>
<td>1570</td>
</tr>
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<td>Use operator splitting</td>
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<td>Solver parameters</td>
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<td>Operator splitting parameters</td>
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<tr>
<td>Reaction time step</td>
<td>200</td>
</tr>
<tr>
<td>Reaction time steps per advection step</td>
<td>10</td>
</tr>
<tr>
<td>Melt settings</td>
<td></td>
</tr>
<tr>
<td>Include melt transport</td>
<td>true</td>
</tr>
<tr>
<td>Heat advection by melt</td>
<td>true</td>
</tr>
</tbody>
</table>

Parameter documentation:

Whether to include the transport of melt into the model or not. If this is set to true, two additional pressures (the fluid pressure and the compaction pressure) will be added to the finite element. Including melt transport in the simulation also requires that there is one compositional field that has the name `porosity`. This field will be used for computing the additional pressures and the melt velocity, and has a different advection equation than other compositional fields, as it is effectively advected with the melt velocity.
<table>
<thead>
<tr>
<th>(Sub)Sections/Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boundary traction model</td>
<td></td>
</tr>
<tr>
<td>Mesh refinement</td>
<td></td>
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<tr>
<td>Postprocess</td>
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<td>Checkpointing</td>
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<td>Compositional fields</td>
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<td>Material model</td>
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<tr>
<td>End time</td>
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<tr>
<td>Heating model</td>
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</tr>
<tr>
<td>List of model names</td>
<td>latent heat</td>
</tr>
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<td>Geometry model</td>
<td></td>
</tr>
<tr>
<td>Gravity model</td>
<td></td>
</tr>
<tr>
<td>Initial temperature model</td>
<td></td>
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<tr>
<td>Initial composition model</td>
<td></td>
</tr>
<tr>
<td>Boundary temperature model</td>
<td></td>
</tr>
<tr>
<td>Boundary composition model</td>
<td></td>
</tr>
<tr>
<td>Boundary velocity model</td>
<td></td>
</tr>
</tbody>
</table>

Parameter documentation:

`latent heat`: Implementation of a standard model for latent heat.

`latent heat melt`: Implementation of a standard model for latent heat of melting. This assumes that there is a compositional field called porosity, and it uses the reaction term of this field (the fraction of material that melted in the current time step) multiplied by a constant entropy change for melting all of the material as source term of the heating model.

If there is no field called porosity, the heating terms are 0.
Model geometry

Gravity pointing downward

105 km

70 km
### Geometry

```xml
<Sections/Parameters>
  <Geometry model>
    <Model name> box </Model name>
    <Box>
      <X extent> 105000 </X extent>
      <Y extent> 70000 </Y extent>
      <X repetitions> 3 </X repetitions>
      <Y repetitions> 2 </Y repetitions>
    </Box>
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    </Gravity model>
  </Geometry model>
  <Initial temperature model>
  </Initial temperature model>
  <Initial composition model>
  </Initial composition model>
  <Boundary temperature model>
  </Boundary temperature model>
  <Boundary composition model>
  </Boundary composition model>
  <Boundary velocity model>
  </Boundary velocity model>
</Sections/Parameters>
```

**Parameter documentation:**

`box`: A box geometry parallel to the coordinate directions. The extent of the box in each coordinate direction is set in the parameter file. The box geometry labels its 2*dim sides as follows: in 2d, boundary indicators 0 through 3 denote the left, right, bottom and top boundaries; in 3d, boundary indicators 0 through 5 indicate left, right, front, back, bottom and top boundaries (see also the documentation of the deal.II class `GeometryInfo`). You can also use symbolic names `"left"`, `"right"`, etc., to refer to these boundaries in input files. It is also possible to add initial topography to the box model. Note however that this is done after the last initial adaptive refinement cycle. Also, initial topography is supposed to be small, as it is not taken into account when depth or a representative point is computed.
Mesh

Coarse grid (X repetitions, Y repetitions)

70 km
Mesh

Coarse grid (X repetitions, Y repetitions)
1 global refinement

70 km
Mesh

Coarse grid (X repetitions, Y repetitions)
2 global refinements

70 km
Mesh

Coarse grid (X repetitions, Y repetitions)
2 global refinements + 1 adaptive refinement

70 km
Mesh refinement

Choose the resolution based on:
The presence of melt | the compaction length
Another option here would be to use the “compaction length” refinement.
Material properties

Melting and freezing are faster than advection

Melt is less dense than the solid

\[ k_\phi = k_0 \phi^3 \]

\[ \eta(\phi, T) = \eta_0 e^{\alpha(\phi - \phi_0)} \]

\[ \xi(\phi, T) = \xi_0 \frac{\phi_0}{\phi} \]

Permeability, shear and compaction viscosities depend on the porosity

Peridotite melting (after Katz et al., 2003)
Material properties

Subsections/Parameters | Value
--- | ---
Compositional fields
  - Number of fields: 2
  - Names of fields: porosity, peridotite
Material model
  - Model name: melt simple
  - Reference permeability: 1e-07
  - Melt extraction depth: 0
  - Freezing rate: 0.005
  - Melting time scale for operator splitting: 200
  - End time: 8000000

Parameter documentation:

`melt simple`: A material model that implements a simple formulation of the material parameters required for the modelling of melt transport, including a source term for the porosity according to the melting model for dry peridotite of \cite{KSL2003}. This also includes a computation of the latent heat of melting (if the `latent heat` heating model is active).

Most of the material properties are constant, except for the shear, viscosity $\eta$, the compaction viscosity $\chi$, and the permeability $k$, which depend on the porosity; and the solid and melt densities, which depend on temperature and pressure:
### Material properties

<table>
<thead>
<tr>
<th>(Sub)Sections/Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melt simple</td>
<td></td>
</tr>
<tr>
<td>Reference solid density</td>
<td>3000</td>
</tr>
<tr>
<td>Reference melt density</td>
<td>2500</td>
</tr>
<tr>
<td>Reference temperature</td>
<td>293</td>
</tr>
<tr>
<td>Reference shear viscosity</td>
<td>5e+20</td>
</tr>
<tr>
<td>Reference bulk viscosity</td>
<td>1e+22</td>
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<tr>
<td>Reference melt viscosity</td>
<td>10</td>
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<tr>
<td>Exponential melt weakening factor</td>
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<tr>
<td>Maximum temperature-induced viscosity variation</td>
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<tr>
<td>Thermal viscosity exponent</td>
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</tr>
<tr>
<td>Thermal bulk viscosity exponent</td>
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<tr>
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<td>Thermal expansion coefficient</td>
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<tr>
<td>Reference permeability</td>
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<tr>
<td>Melt extraction depth</td>
<td>0</td>
</tr>
<tr>
<td>Solid compressibility</td>
<td>0</td>
</tr>
</tbody>
</table>

**Parameter documentation:**

The value of the constant viscosity $\eta_0$ of the solid matrix. This viscosity may be modified by both temperature and porosity dependencies. Units: $Pa \, s$. 
Initial conditions

Cold top boundary layer

- No melt is present
- No depletion / enrichment

Constant temperature = potential temperature

105 km

70 km
Boundary conditions

prescribed velocity, no outflow
prescribed temperature = 293 K

free slip

prescribed traction: lithostatic pressure
prescribed temperature = 1570 K
zero porosity, zero depletion
### Boundary conditions

<table>
<thead>
<tr>
<th>SubSections/Parameters</th>
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</tr>
</thead>
<tbody>
<tr>
<td>Boundary temperature model</td>
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</tr>
<tr>
<td>List of model names</td>
<td>box</td>
</tr>
<tr>
<td>Fixed temperature boundary indicators</td>
<td>top, bottom</td>
</tr>
<tr>
<td>Box</td>
<td></td>
</tr>
<tr>
<td>Bottom temperature</td>
<td>1570</td>
</tr>
<tr>
<td>Top temperature</td>
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<td>Boundary composition model</td>
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<td>List of model names</td>
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<td>Fixed composition boundary indicators</td>
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<td>Boundary velocity model</td>
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<tr>
<td>Prescribed velocity boundary indicators</td>
<td>top: function</td>
</tr>
<tr>
<td>Tangential velocity boundary indicators</td>
<td>left</td>
</tr>
<tr>
<td>Function</td>
<td></td>
</tr>
<tr>
<td>Variable names</td>
<td>x,Z</td>
</tr>
<tr>
<td>Function expression</td>
<td>if(x&lt;x0,(1-(x/x0-1)*(x/x0-1))*u0,u0); 0</td>
</tr>
<tr>
<td>Function constants</td>
<td>u0=0.03, x0=10000</td>
</tr>
</tbody>
</table>

**Parameter documentation:**

`box`: A model in which the temperature is chosen constant on the sides of a box which are selected by the parameters Left/Right/Top/Bottom/Front/Back temperature.

`box with lithosphere boundary indicators`: A model in which the temperature is chosen constant on all the sides of a box. Additional boundary indicators are added to the lithospheric parts of the vertical boundaries. This model is to be used with the 'Two Merged Boxes' Geometry Model.
Boundary conditions

Parameter documentation:

A comma separated list denoting those boundaries on which a traction force is prescribed, i.e., where known external forces act, resulting in an unknown velocity. This is often used to model "open" boundaries where we only know the pressure. This pressure then produces a force that is normal to the boundary and proportional to the pressure.

The format of valid entries for this parameter is that of a map given as "key1 [selector]: value1, key2 [selector]: value2, key3: value3, ..." where each key must be a valid boundary indicator (which is either an integer or the symbolic name the geometry model in use may have provided for this part of the boundary) and each value must be one of the currently implemented boundary traction models. "selector" is an optional string given as a subset of the letters "xyzt" that allows

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<td>Solver parameters</td>
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<td>Melt settings</td>
<td></td>
</tr>
<tr>
<td>Boundary traction model</td>
<td></td>
</tr>
<tr>
<td>Prescribed traction boundary indicators</td>
<td>right: initial lithostatic pressure, bottom: initial lithostatic pressure</td>
</tr>
<tr>
<td>Initial lithostatic pressure</td>
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<tr>
<td>Representative point</td>
<td>105000, 70000</td>
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<td>Mesh refinement</td>
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<td></td>
</tr>
<tr>
<td>End time</td>
<td>8000000</td>
</tr>
<tr>
<td>Heating model</td>
<td></td>
</tr>
</tbody>
</table>
We have to iterate between Stokes and advection system! We want to solve reactions separately because they are much faster.
• The output file is located in: 
/home/ubuntu/Desktop/output_mid_ocean_ridge
Paraview: Plot contours
Paraview: Plot glyphs

This property indicates the name of the vector array on which to operate. The indicated array may be used for scaling and/or orienting the glyphs. (See the SetScaleMode and SetOrient properties.)
Results
Model evolution
Results: chemical composition

- Vertical profile through the model
  \textit{(Paraview: Filters \Rightarrow Plot over line)}

- Enriched crust
- Depleted lithosphere
- Crustal thickness: \(~8\) km
Things to play with

Vary:

- Spreading rate
- Shear viscosity
- Permeability
- Compaction viscosity

Katz, 2010
Things to play with

Vary:

• Spreading rate
• Shear viscosity
• Permeability
• Compaction viscosity

Katz, 2008
Things to play with

Ideas: Making the model more realistic

• Temperature-dependent rheology
• Dislocation creep & brittle failure
• Free surface
• Prescribe force on the sides instead of surface velocity
• Other heating processes (Adiabatic heating, shear heating, ...)
• Melting parametrization: use thermodynamics software?
More information

• ASPECT manual:  
  http://www.math.clemson.edu/~heister/manual.pdf

  https://doi.org/10.1093/gji/ggw329

• Ask on the mailing list:  
  http://lists.geodynamics.org/cgi-bin/mailman/listinfo/aspect-devel