ASPECT tutorial
Part II: Melt transport

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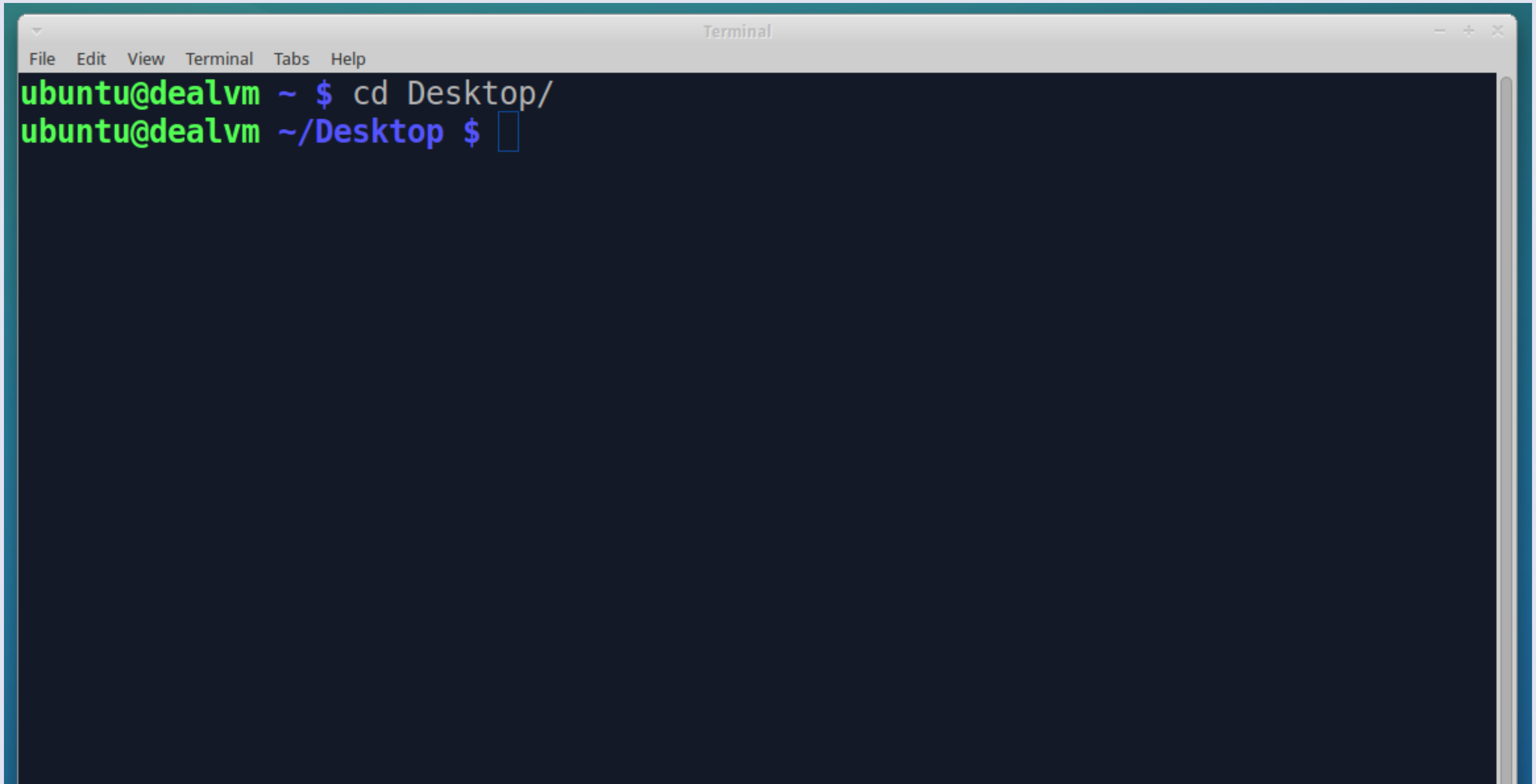
Rene Gassmöller, John Naliboff

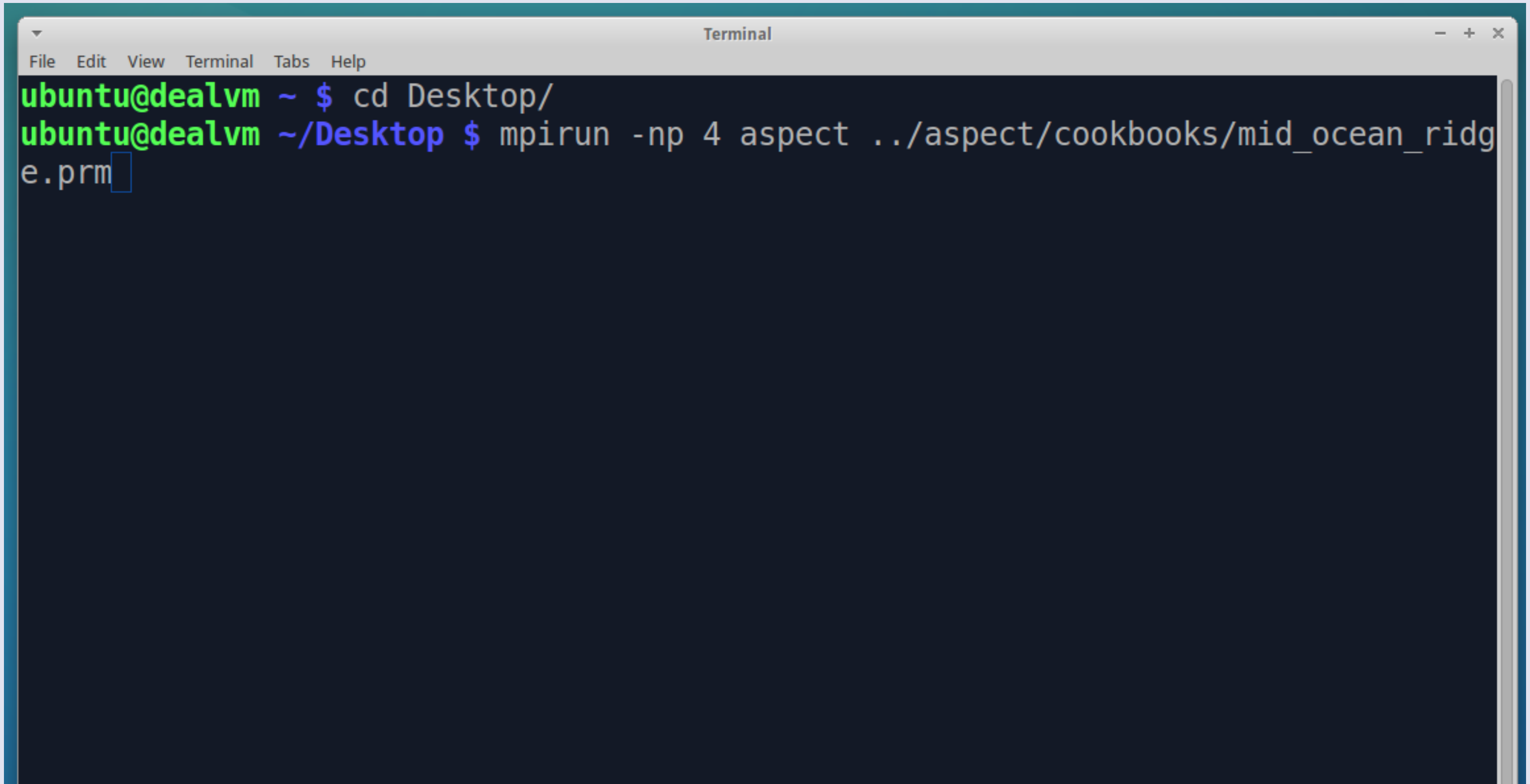
Starting the model…

- 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...

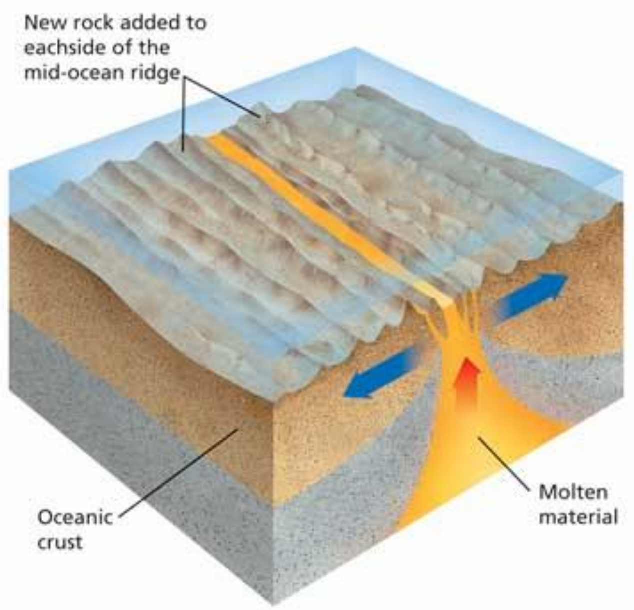
- This should give you output like this
- We will let this model run and come back later

```
Terminal
File  Edit  View  Terminal  Tabs  Help
ubuntu@dealvm ~ $ cd Desktop/
ubuntu@dealvm ~/Desktop $ aspect ../aspect/cookbooks/mid_ocean_ridge.prm
-----------------------------------------------------------------------------
-- This is ASPECT, the Advanced Solver for Problems in Earth's ConvecTion.
--     . version 2.0.0
--     . using deal.II 9.0.0-rc3 (dealii-9.0, 3975bad)
--     . using Trilinos 12.10.1
--     . using p4est 2.0.0
--     . running in OPTIMIZED mode
--     . running with 1 MPI process
-- How to cite ASPECT: https://aspect.geodynamics.org/cite.html
-----------------------------------------------------------------------------



-----------------------------------------------------------------------------
The output directory <output_mid_ocean_ridge/> provided in the input file appear
s not to exist.
ASPECT will create it for you.
```

Outline

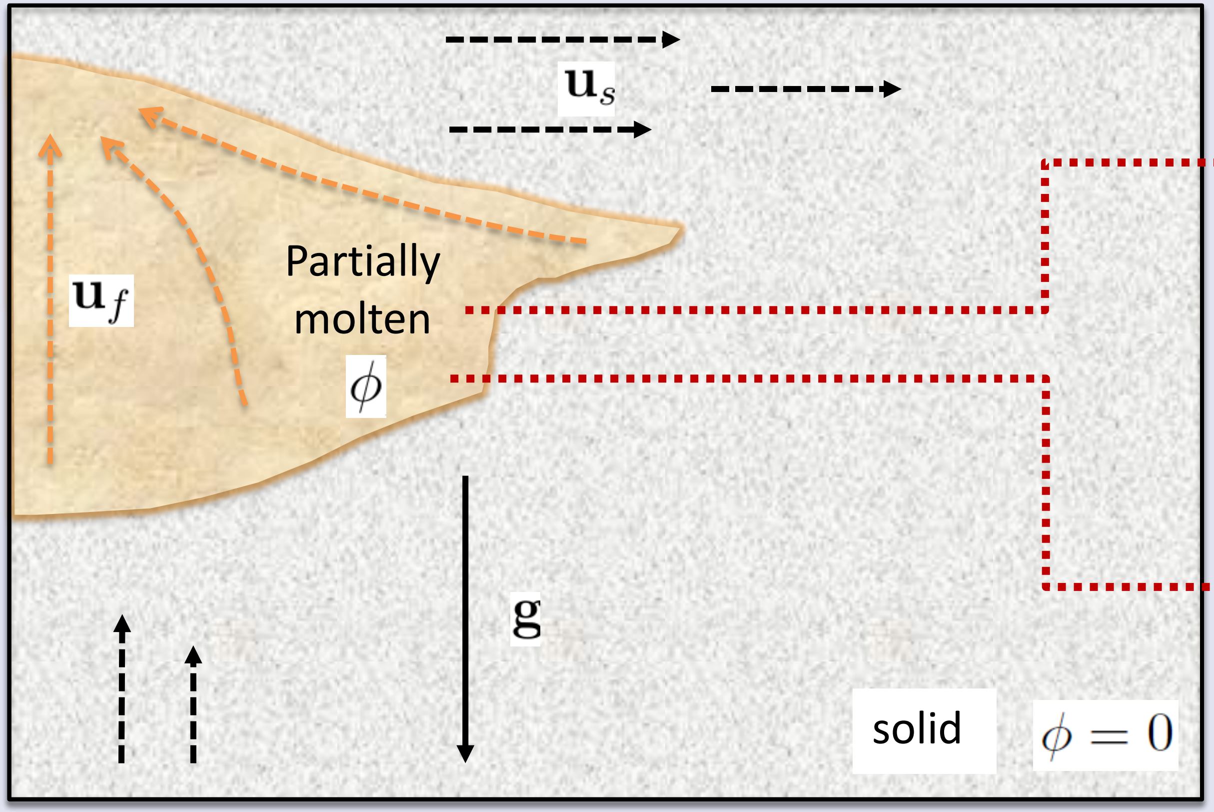
1. Theory
2. Methods
3. Example
4. Playtime

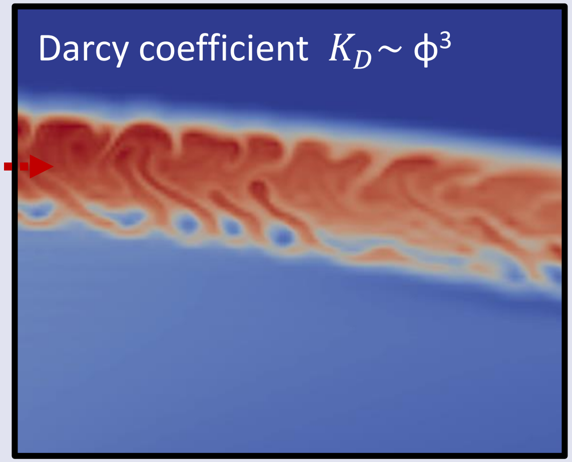
Mid-ocean ridges

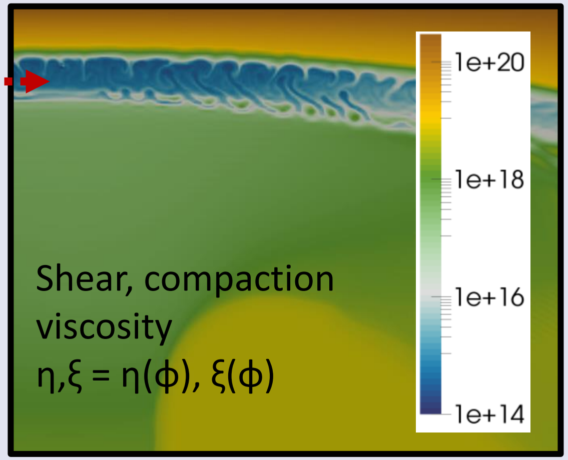


From http://www.phschool.com

The problem







ρ	density	ξ^*	compaction viscosity
η^*	shear viscosity	K_D	Darcy coefficient

Additional material

Excellent introduction:

Spiegelman, M., Katz, R., & Simpson, G. (2007). An Introduction and Tutorial to the "McKenzie Equations" for magma migration.

http://www.deep-earth.org/2010/Spiegelman-melt.pdf

Very comprehensive lecture notes:

Katz, R. F. (2011). An introduction to coupled magma/mantle dynamics.

http://foalab.earth.ox.ac.uk/files/IntroMagmaLectures.pdf

Equations: Mantle convection

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

Mass conservation

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

Momentum conservation

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

u_s, solid velocity
p pressure
ρ density
g gravity

Energy conservation

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

Equations: Magma/mantle dynamics

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

Mass conservation

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

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

Momentum conservation

$$\phi\left(\mathbf{u}_f - \mathbf{u}_s\right) = -K_D\left(\nabla p_f - \rho_f \mathbf{g}\right)$$

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

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

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

$u_{s,f}$ solid, fluid velocity
ϕ porosity
p_f fluid pressure
p_c compaction pressure
$\rho_{s,f}$ density
g gravity
Γ 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.

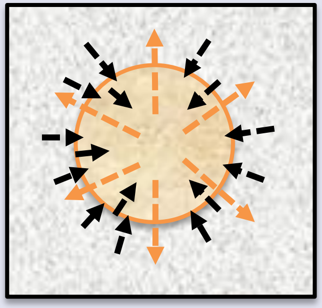
The difference between solid and melt velocity depends on the permeability and pressure gradients in the melt.

Momentum conservation

$$\phi\left(\mathbf{u}_f - \mathbf{u}_s\right) = -K_D\left(\nabla p_f - \rho_f \mathbf{g}\right)$$

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

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

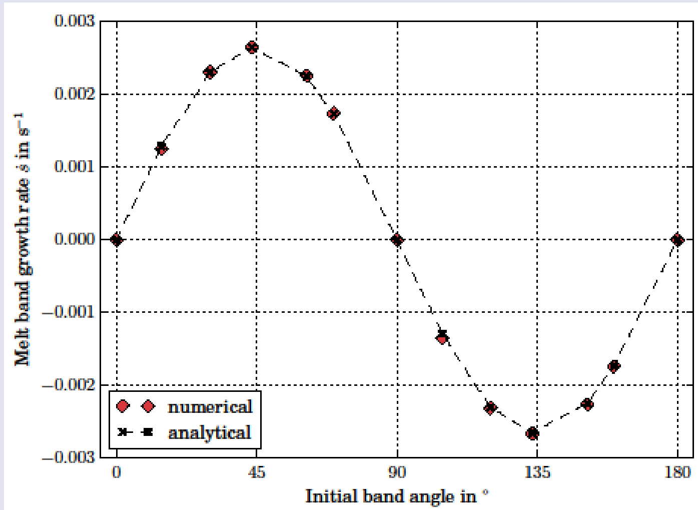
- Separation flux:

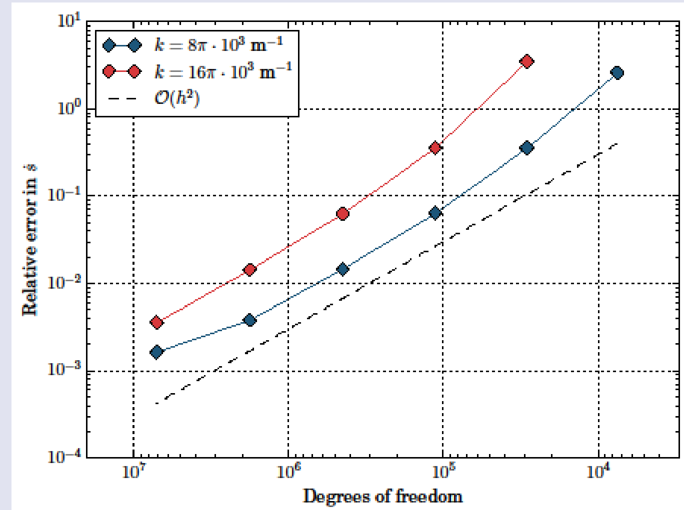
$$\phi w = \frac{k\Delta\rho g}{\eta_f}$$

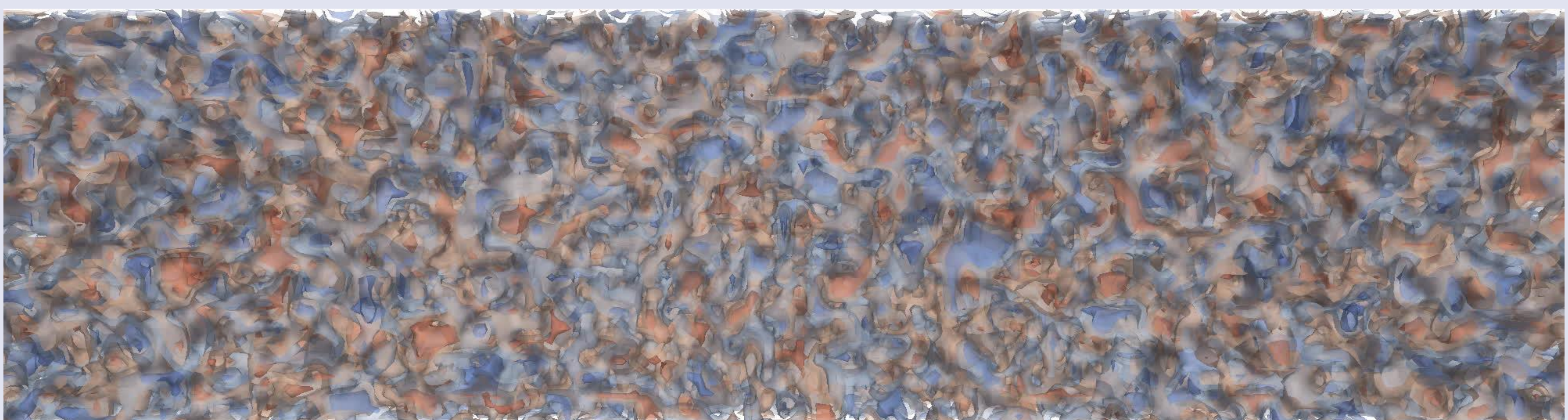
is an estimate of the (gravity drive) melt flux relative to the solid

Shear bands

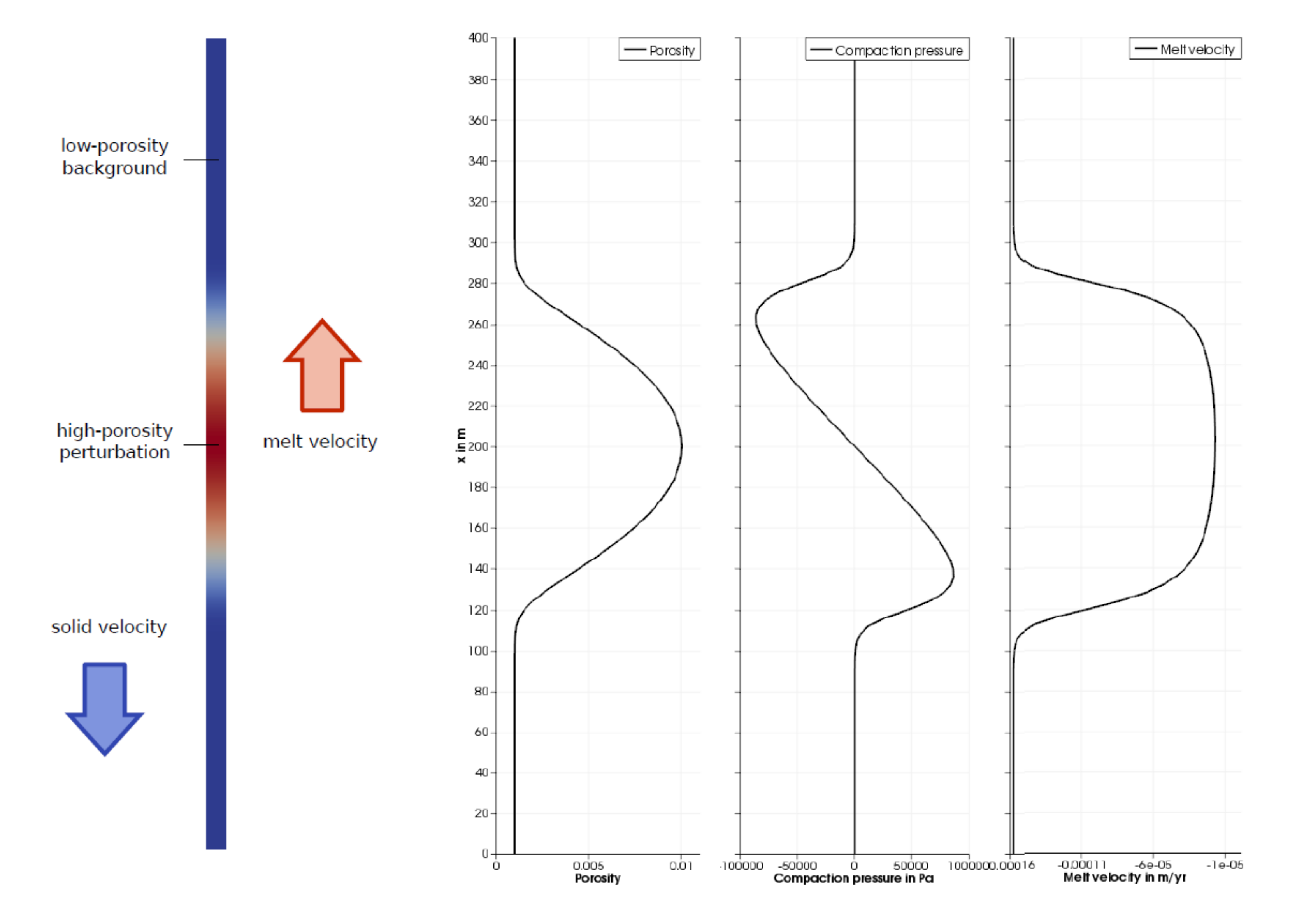
Magmatic shear bands







Solitary waves



Methods

PDE system

CIG COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

Eliminating $\mathbf{u}_f$ and introducing the compaction pressure p_c leads to:

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

$$\begin{aligned}\nabla \cdot \mathbf{u}_s - \nabla \cdot K_D \nabla p_f - K_D \nabla p_f \cdot \frac{\nabla \rho_f}{\rho_f} = &-\nabla \cdot (K_D \rho_f \mathbf{g}) \\ &+ \Gamma \left(\frac{1}{\rho_f} - \frac{1}{\rho_s}\right) \\ &- \frac{\phi}{\rho_f}\mathbf{u}_s \cdot \nabla \rho_f - (\mathbf{u}_s \cdot \mathbf{g})(1-\phi)\kappa_s \rho_s \\ &- K_D \mathbf{g} \cdot \nabla \rho_f,\end{aligned}$$

$$\nabla \cdot \mathbf{u}_s + \frac{p_c}{\xi} = 0.$$

Melt advection

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

PDE system

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

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

$$\begin{aligned}\nabla\cdot\mathbf{u}_s - \nabla\cdot K_D\nabla p_f - K_D\nabla p_f\cdot\frac{\nabla\rho_f}{\rho_f} &= -\nabla\cdot(K_D\rho_f\mathbf{g}) \\ &\quad + \Gamma\left(\frac{1}{\rho_f} - \frac{1}{\rho_s}\right) \\ &\quad - \frac{\phi}{\rho_f}\mathbf{u}_s\cdot\nabla\rho_f - (\mathbf{u}_s\cdot\mathbf{g})(1-\phi)\kappa_s\rho_s \\ &\quad - K_D\mathbf{g}\cdot\nabla\rho_f,\end{aligned}$$

$$\nabla\cdot\mathbf{u}_s + \frac{p_c}{\xi} = 0.$$

Discretization yields the linear system

$$\begin{pmatrix}\mathbf{A} & \mathbf{B}^T & \mathbf{B}^T \\ \mathbf{B} & \mathbf{N} & \mathbf{0} \\ \mathbf{B} & \mathbf{0} & \mathbf{K}\end{pmatrix}\begin{pmatrix}\mathbf{U}_s \\ \mathbf{P}_f \\ \mathbf{P}_c\end{pmatrix} = \begin{pmatrix}\mathbf{F} \\ \mathbf{G} \\ \mathbf{0}\end{pmatrix}$$

New formulation

Inspired by:

SIAM J. Sci. Comput. Vol. 39, No. 2, pp. B375–B402 © 2017 Society for Industrial and Applied Mathematics

MIXED METHODS FOR TWO-PHASE DARCY–STOKES MIXTURES OF PARTIALLY MELTED MATERIALS WITH REGIONS OF ZERO POROSITY*

TODD ARBOGAST†, MARC A. HESSE‡, AND ABRAHAM L. TAICHER§

$$\begin{pmatrix} \mathbf{A} & \mathbf{B}^T & \mathbf{B}^T \\ \mathbf{B} & \mathbf{N} & \mathbf{0} \\ \mathbf{B} & \mathbf{0} & \mathbf{K} \end{pmatrix} \begin{pmatrix} \mathbf{U}_s \\ \mathbf{P}_f \\ \mathbf{P}_c \end{pmatrix} = \begin{pmatrix} \mathbf{F} \\ \mathbf{G} \\ \mathbf{0} \end{pmatrix}$$

replace p_c with $\bar{p}_c$,
where $p_c = \sqrt{K_D} \cdot \bar{p}_c$

$$\begin{pmatrix} \mathbf{A} & \mathbf{B}^T & \sqrt{K_D}\mathbf{B}^T \\ \mathbf{B} & \mathbf{N} & \mathbf{0} \\ \sqrt{K_D}\mathbf{B} & \mathbf{0} & K_D\mathbf{K} \end{pmatrix} \begin{pmatrix} \mathbf{U}_s \\ \mathbf{P}_f \\ \bar{\mathbf{P}}_c \end{pmatrix} = \begin{pmatrix} \mathbf{F} \\ \mathbf{G} \\ \mathbf{0} \end{pmatrix}$$

From R. Grove, PhD thesis

- 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 $\phi \to 0$

New formulation: $\phi \rightarrow 0$

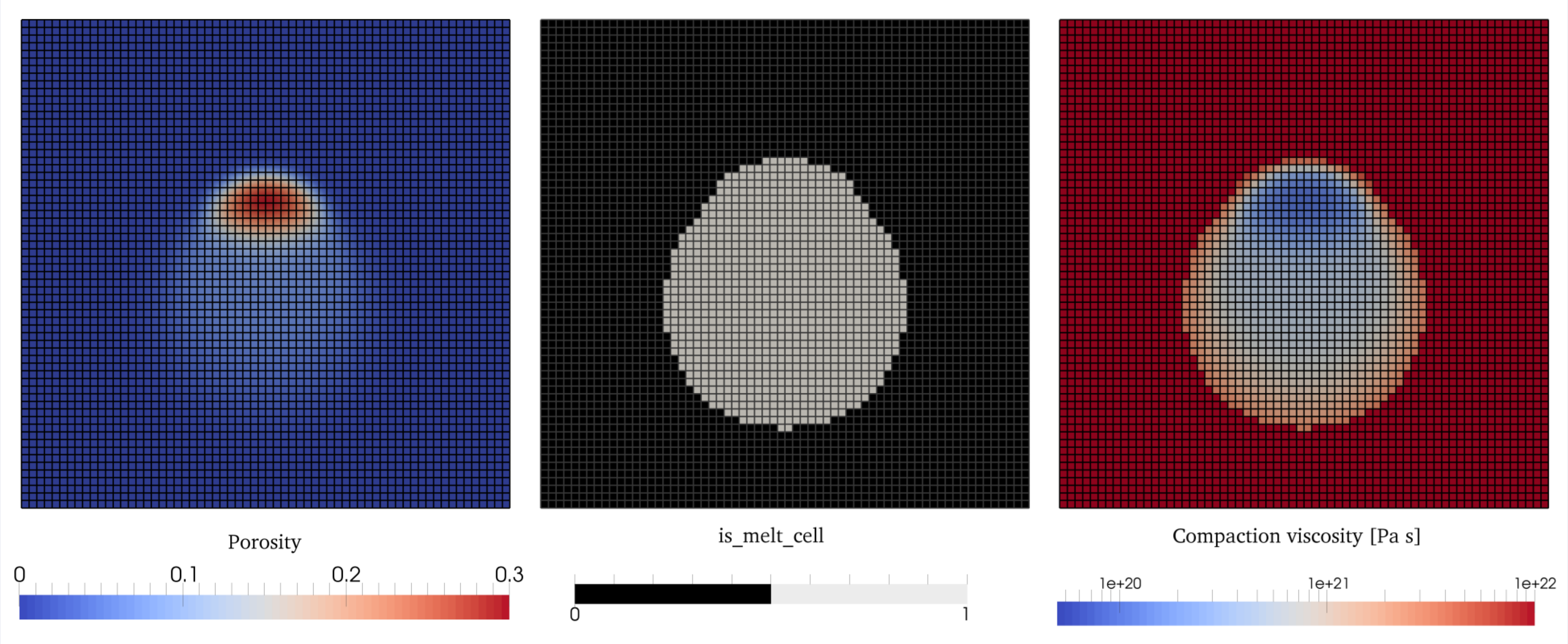
$$\begin{pmatrix} \mathbf{A} & \mathbf{B}^T & \mathbf{B}^T \\ \mathbf{B} & \mathbf{N} & \mathbf{0} \\ \mathbf{B} & \mathbf{0} & \mathbf{K} \end{pmatrix} \begin{pmatrix} \mathbf{U}_s \\ \mathbf{P}_f \\ \mathbf{P}_c \end{pmatrix} = \begin{pmatrix} \mathbf{F} \\ \mathbf{G} \\ \mathbf{0} \end{pmatrix}$$

Stokes system

$$\begin{pmatrix} \mathbf{A} & \mathbf{B}^T & \sqrt{K_D}\mathbf{B}^T \\ \mathbf{B} & \mathbf{N} & \mathbf{0} \\ \sqrt{K_D}\mathbf{B} & \mathbf{0} & K_D\mathbf{K} \end{pmatrix} \begin{pmatrix} \mathbf{U}_s \\ \mathbf{P}_f \\ \bar{\mathbf{P}}_c \end{pmatrix} = \begin{pmatrix} \mathbf{F} \\ \mathbf{G} \\ \mathbf{0} \end{pmatrix}$$

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

Challenge: Reactions

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

- 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

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

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

we first solve the advection equation without reactions

$$\frac{\partial \mathfrak{c}(t)}{\partial t} + \mathbf{u} \cdot \nabla \mathfrak{c}(t) = 0, \text{ obtaining } \Delta \mathfrak{c}_A(t^{n+1}) \text{ from } \mathfrak{c}(t^n),$$

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

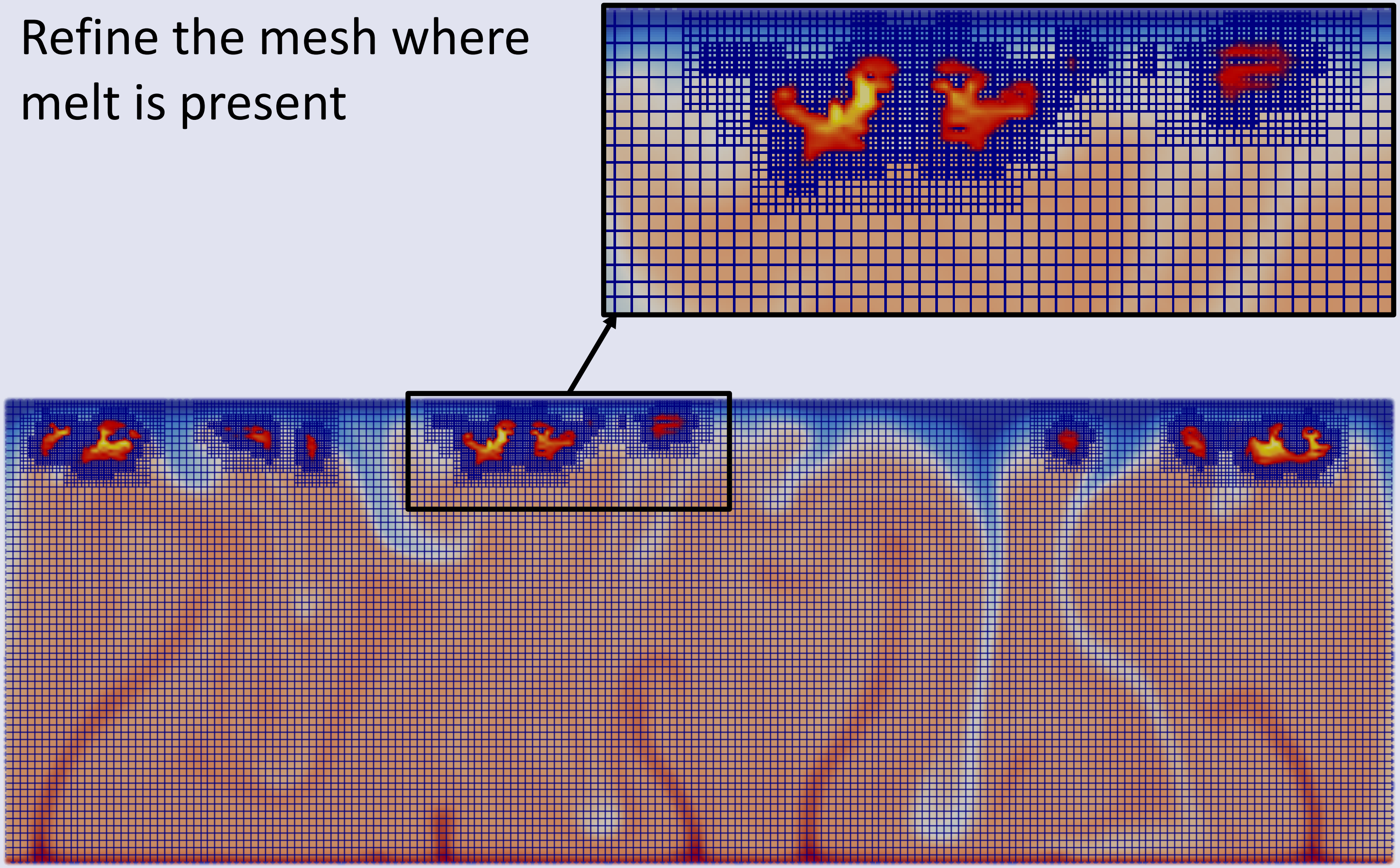
$$\frac{\partial \mathfrak{c}(t)}{\partial t} = q(\mathfrak{c}(t^n) + \Delta \mathfrak{c}_A(t^{n+1}))$$

$$\text{obtaining } \Delta \mathfrak{c}_R(t^{n+1}) \text{ from } \mathfrak{c}(t^n) + \Delta \mathfrak{c}_A(t^{n+1}).$$

- Allows for equilibrium & disequilibrium melting

Adaptive mesh refinement

Refine the mesh where melt is present



Model setup

Ingredients of a Model

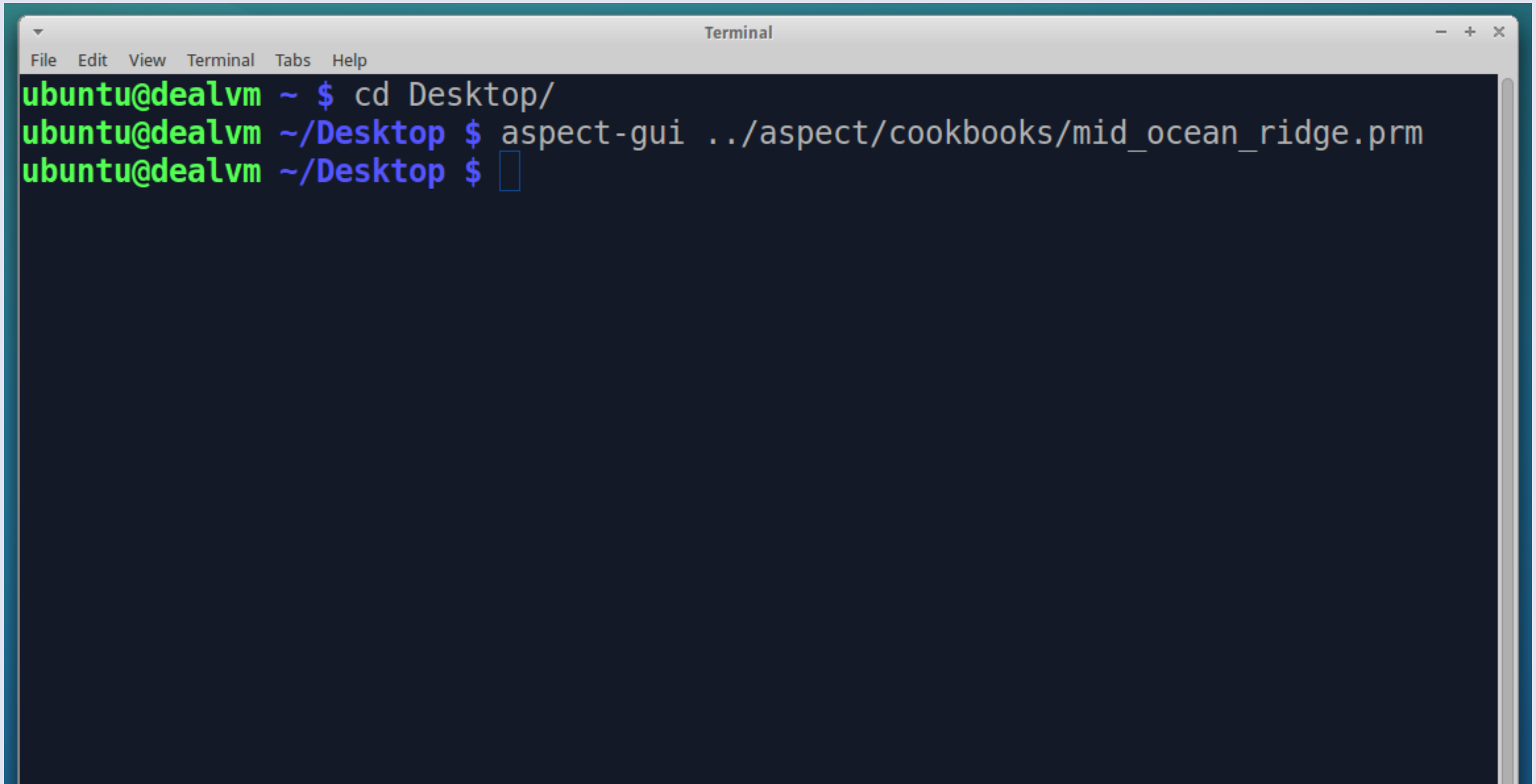
Motivation: What is the question we want to answer?

- 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…

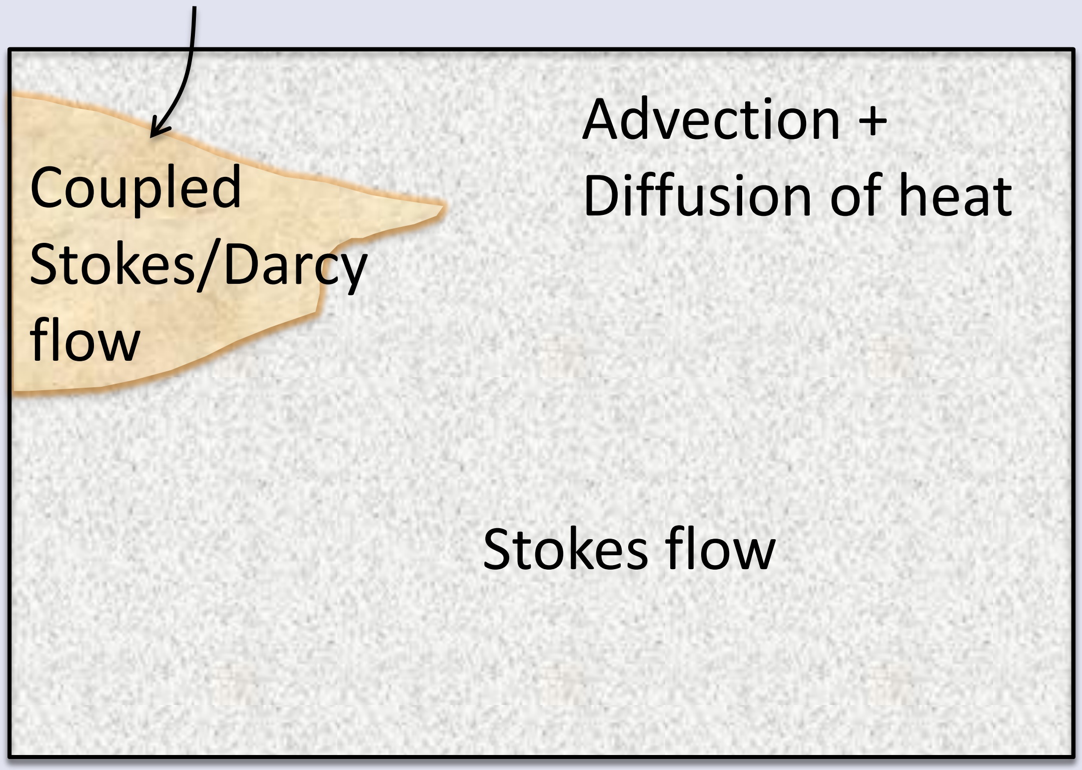
- We will look at the input file in the ASPECT-GUI

```
aspect-gui
../aspect/cookbooks/mid_ocean_ridge.prm
```

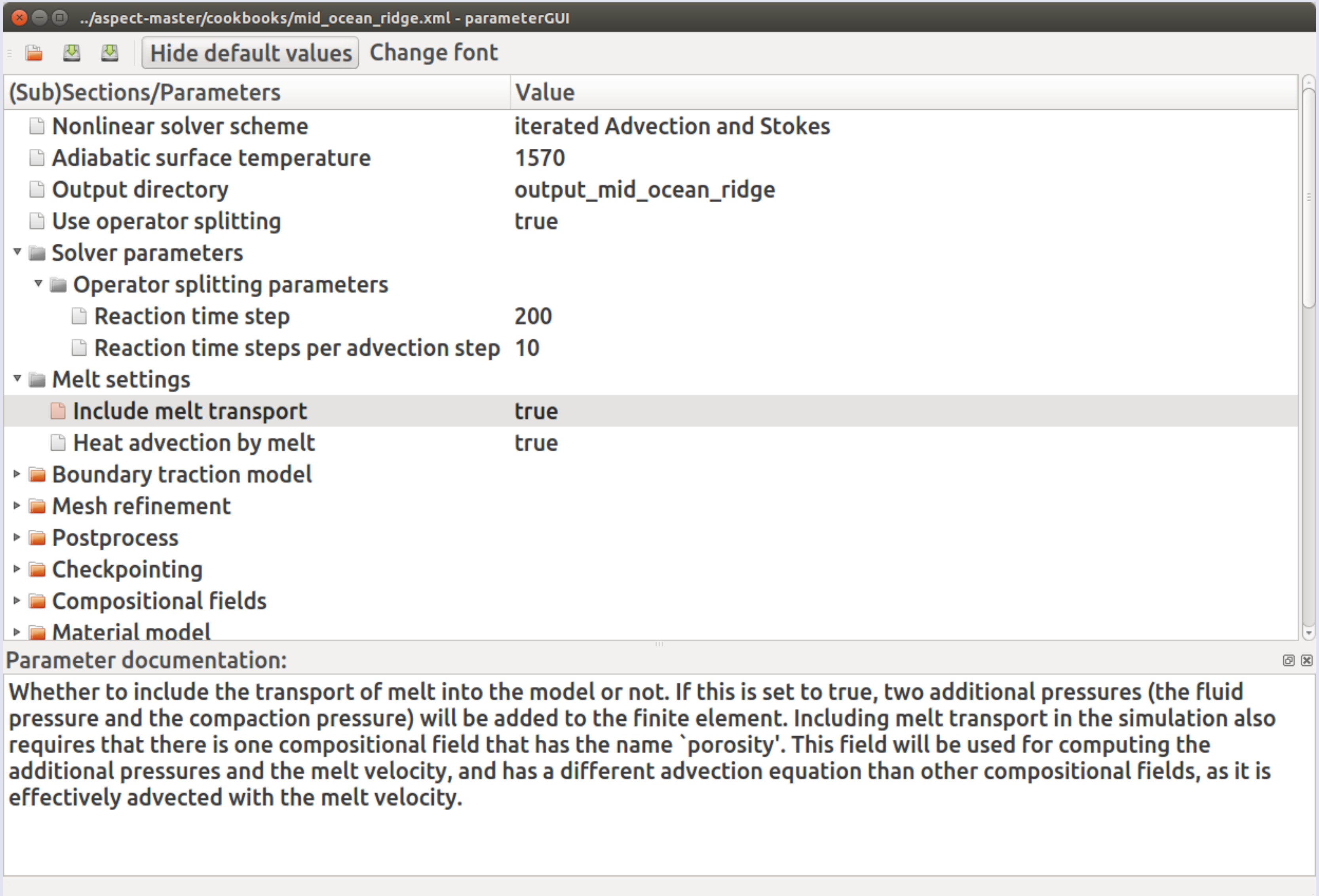


Equations

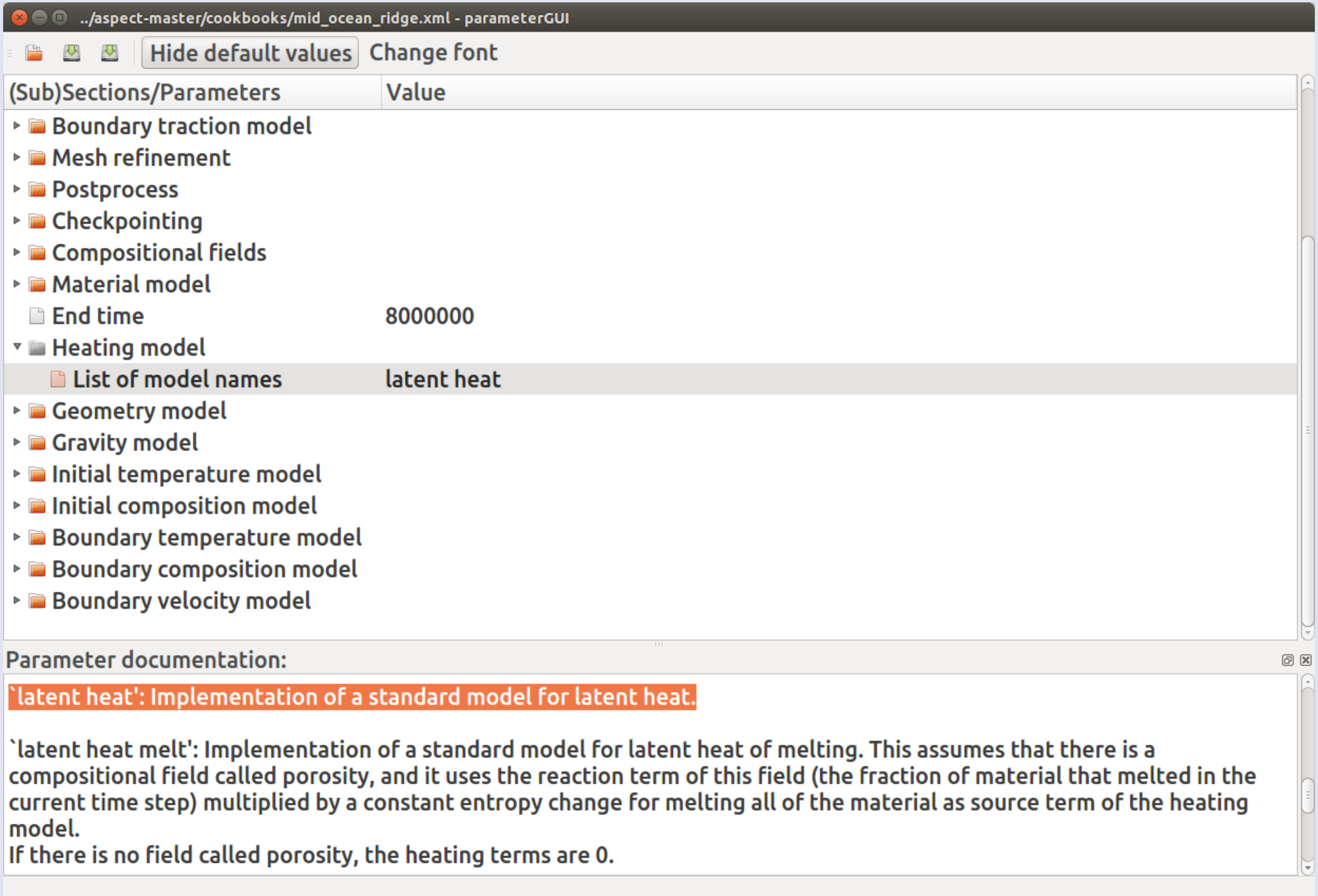
Melting and freezing
reactions + latent heat



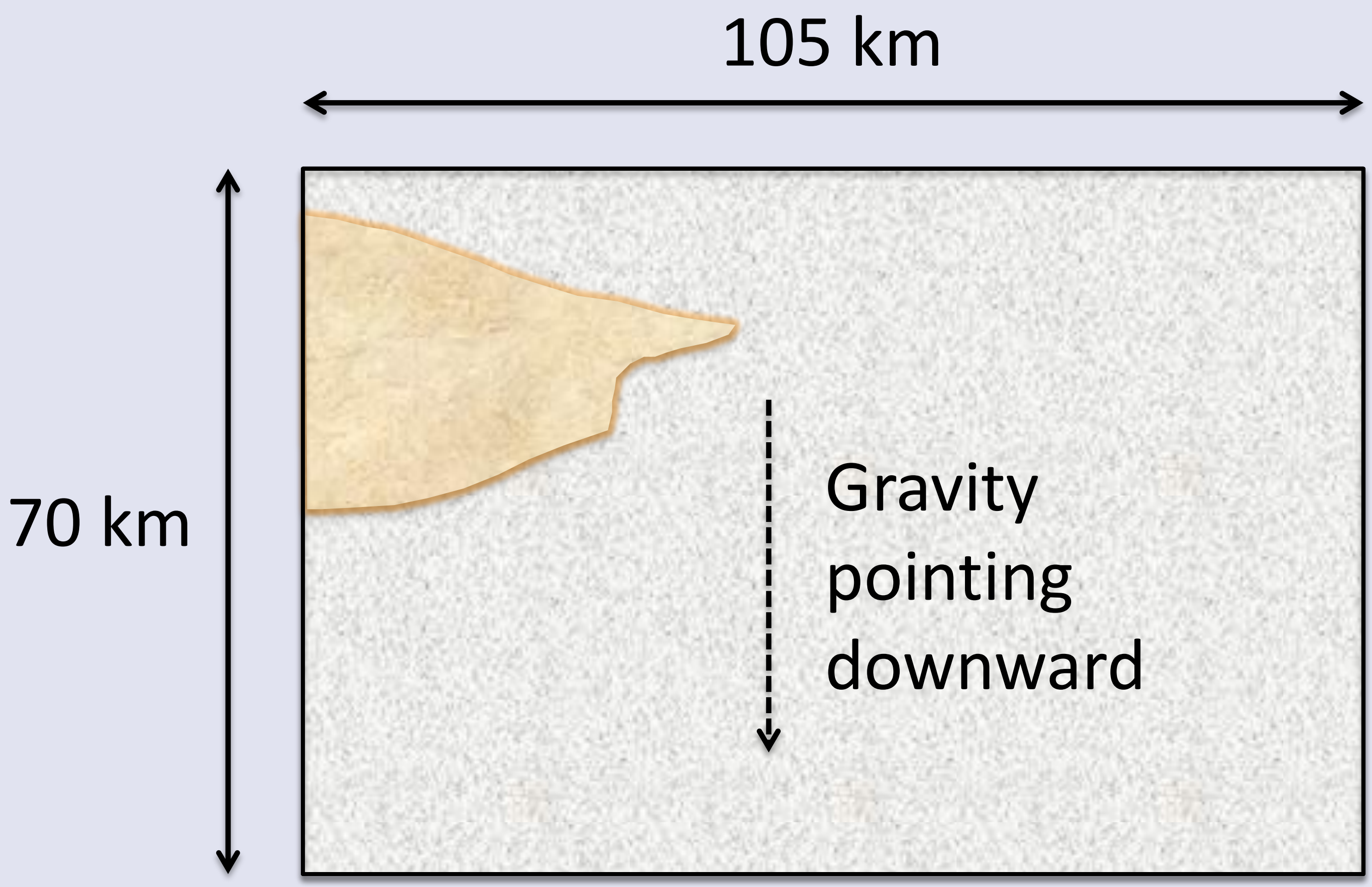
Equations


../aspect-master/cookbooks/mid_ocean_ridge.xml - parameterGUI
Hide default values
Change font
(Sub)Sections/Parameters
Value
Nonlinear solver scheme
iterated Advection and Stokes
Adiabatic surface temperature
1570
Output directory
output_mid_ocean_ridge
Use operator splitting
true
Solver parameters
Operator splitting parameters
Reaction time step
200
Reaction time steps per advection step
10
Melt settings
Include melt transport
true
Heat advection by melt
true
Boundary traction model
Mesh refinement
Postprocess
Checkpointing
Compositional fields
Material model
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.

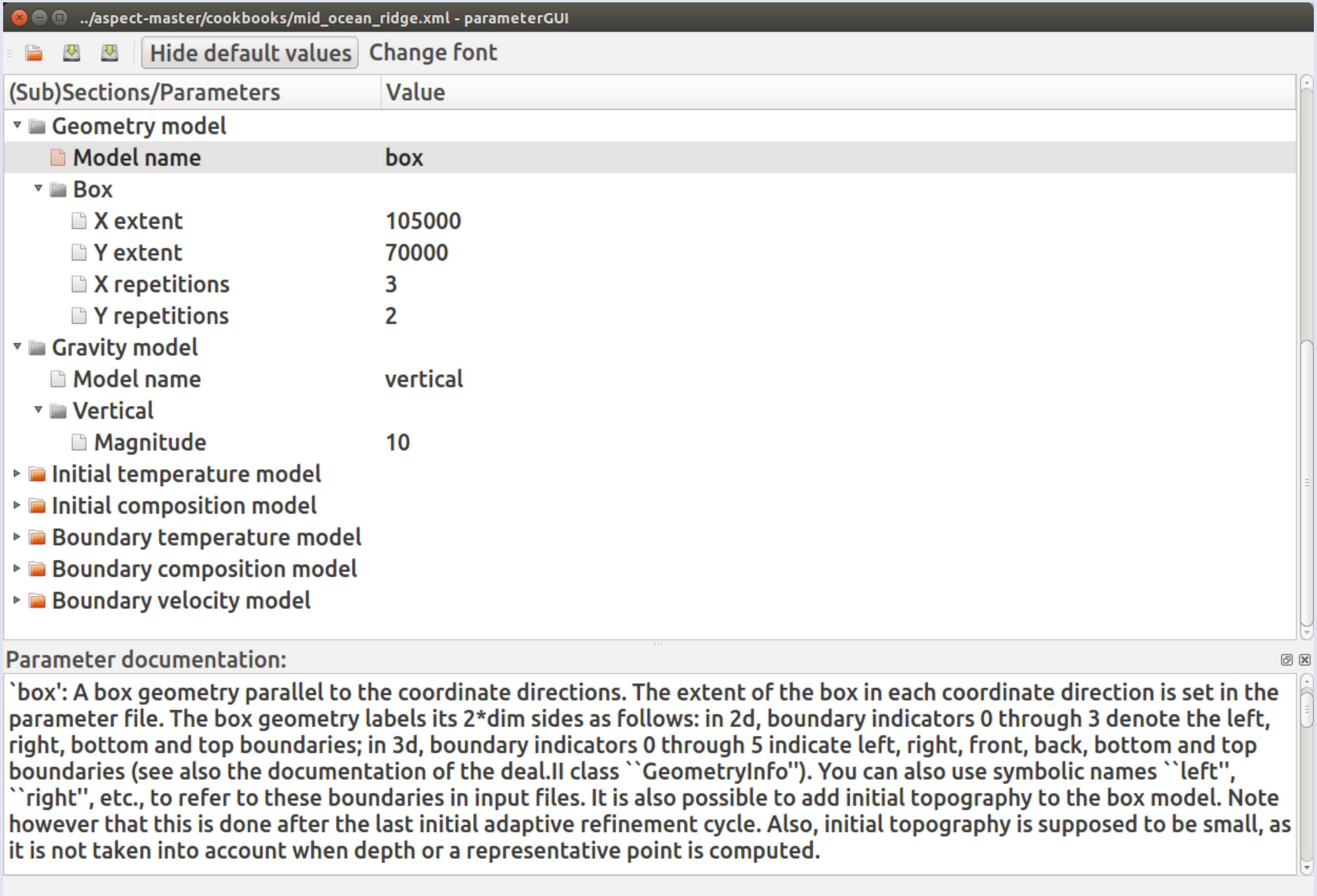
Equations


../aspect-master/cookbooks/mid_ocean_ridge.xml - parameterGUI
Hide default values
Change font
(Sub)Sections/Parameters
Value
Boundary traction model
Mesh refinement
Postprocess
Checkpointing
Compositional fields
Material model
End time
8000000
Heating model
List of model names
latent heat
Geometry model
Gravity model
Initial temperature model
Initial composition model
Boundary temperature model
Boundary composition model
Boundary velocity model
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

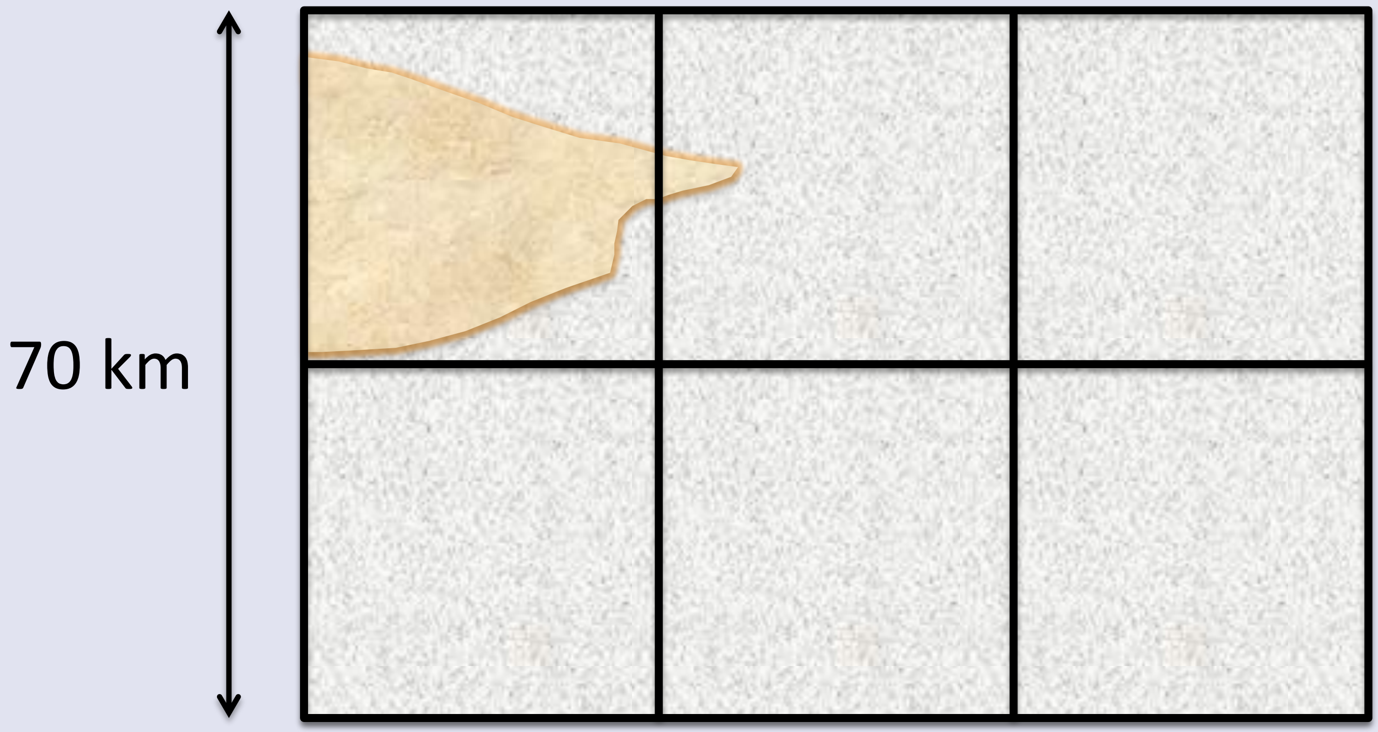


Geometry


../aspect-master/cookbooks/mid_ocean_ridge.xml - parameterGUI
Hide default values
Change font
(Sub)Sections/Parameters
Value
Geometry model
Model name
box
Box
X extent
105000
Y extent
70000
X repetitions
3
Y repetitions
2
Gravity model
Model name
vertical
Vertical
Magnitude
10
Initial temperature model
Initial composition model
Boundary temperature model
Boundary composition model
Boundary velocity model
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)

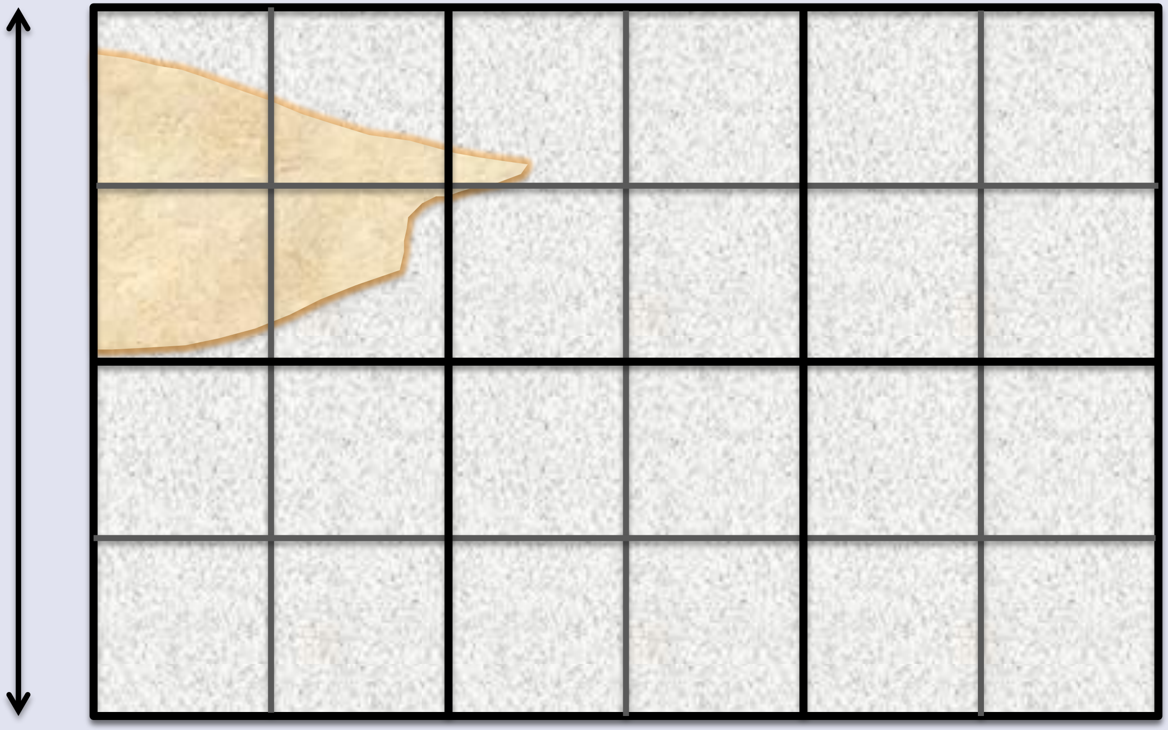


Mesh

Coarse grid (X repetitions, Y repetitions)

1 global refinement

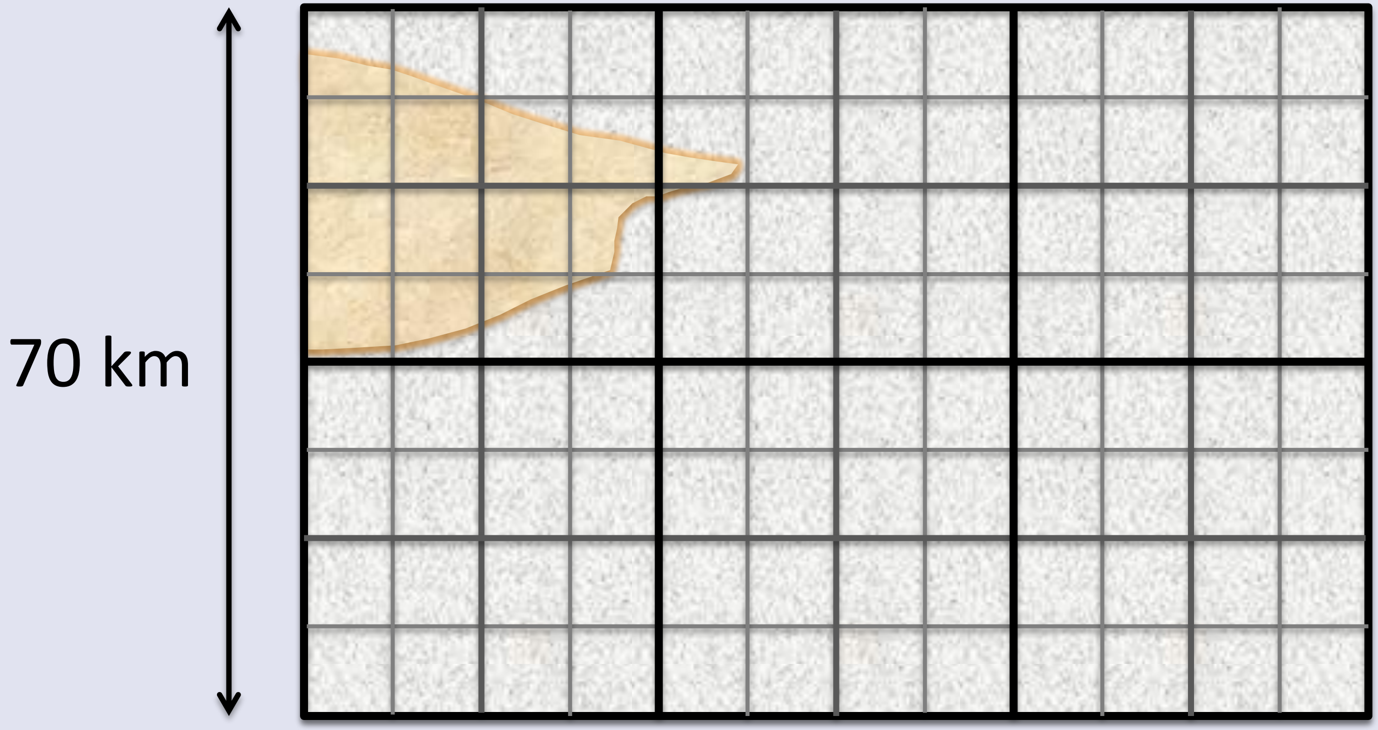
70 km



Mesh

Coarse grid (X repetitions, Y repetitions)

2 global refinements

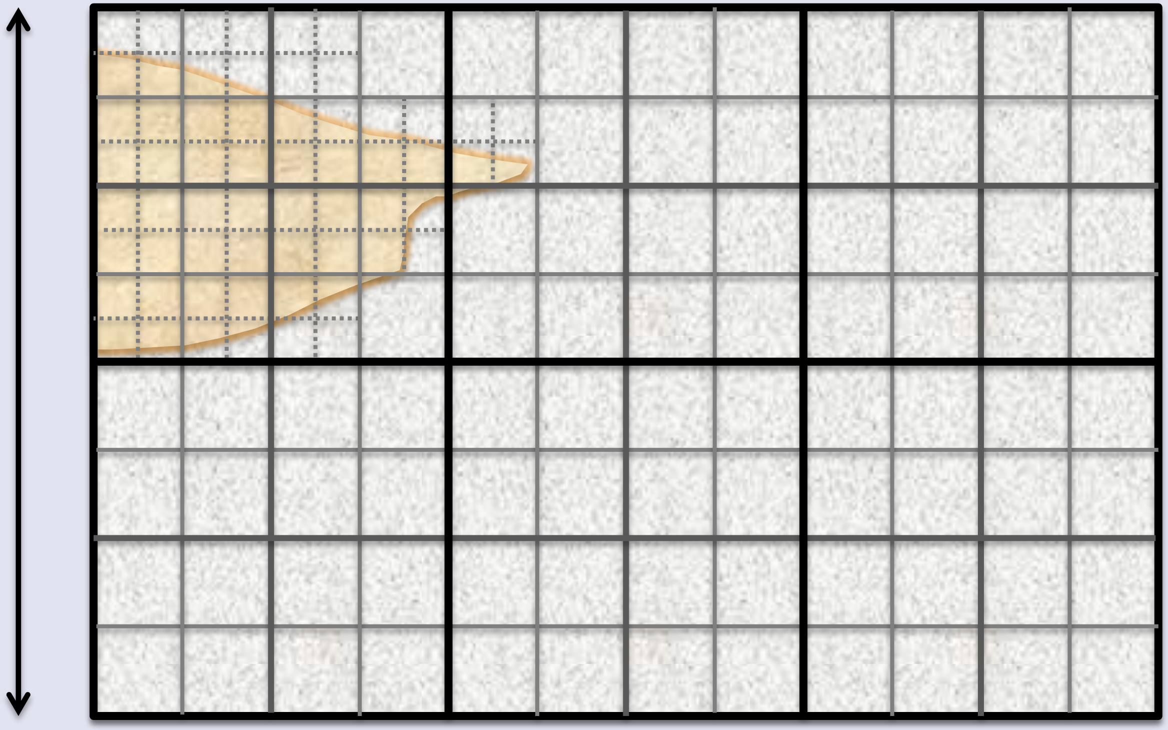


Mesh

Coarse grid (X repetitions, Y repetitions)

2 global refinements + 1 adaptive refinement

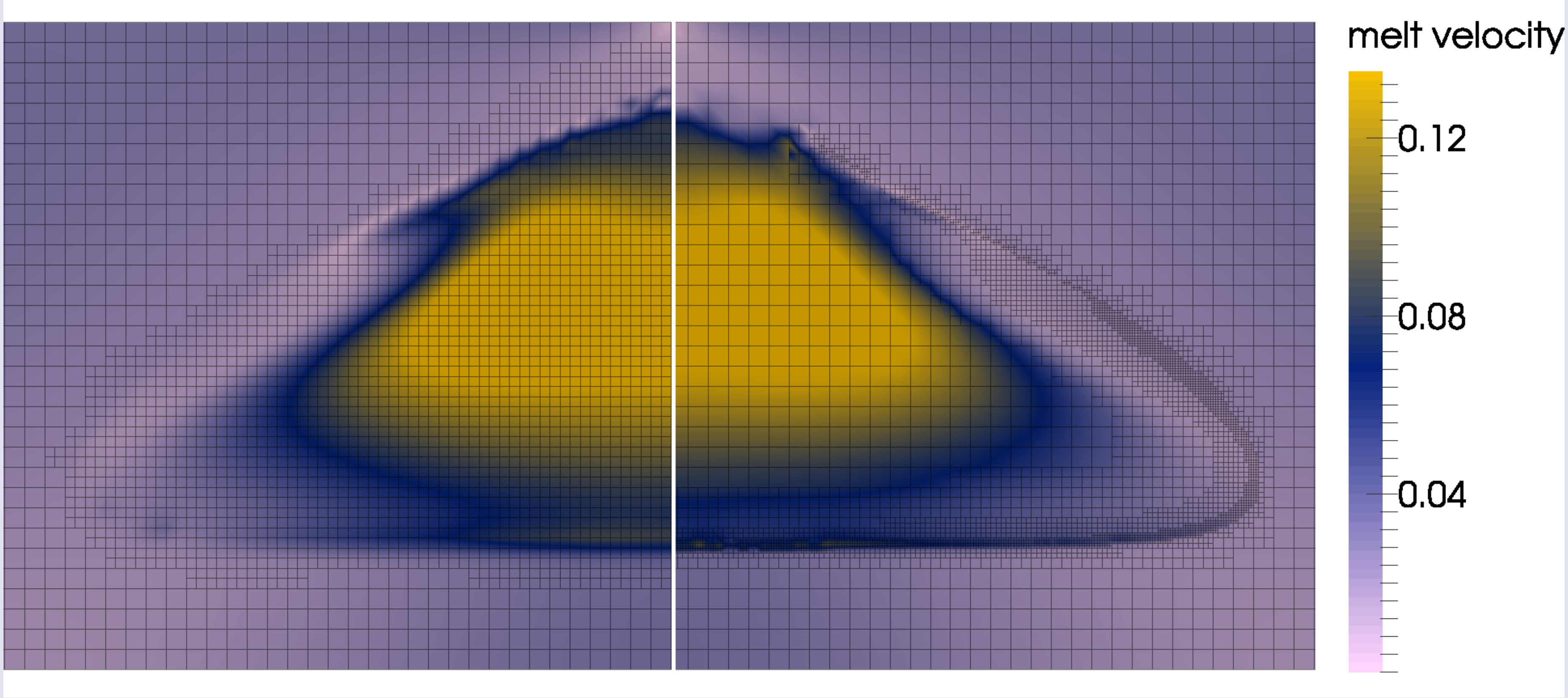
70 km



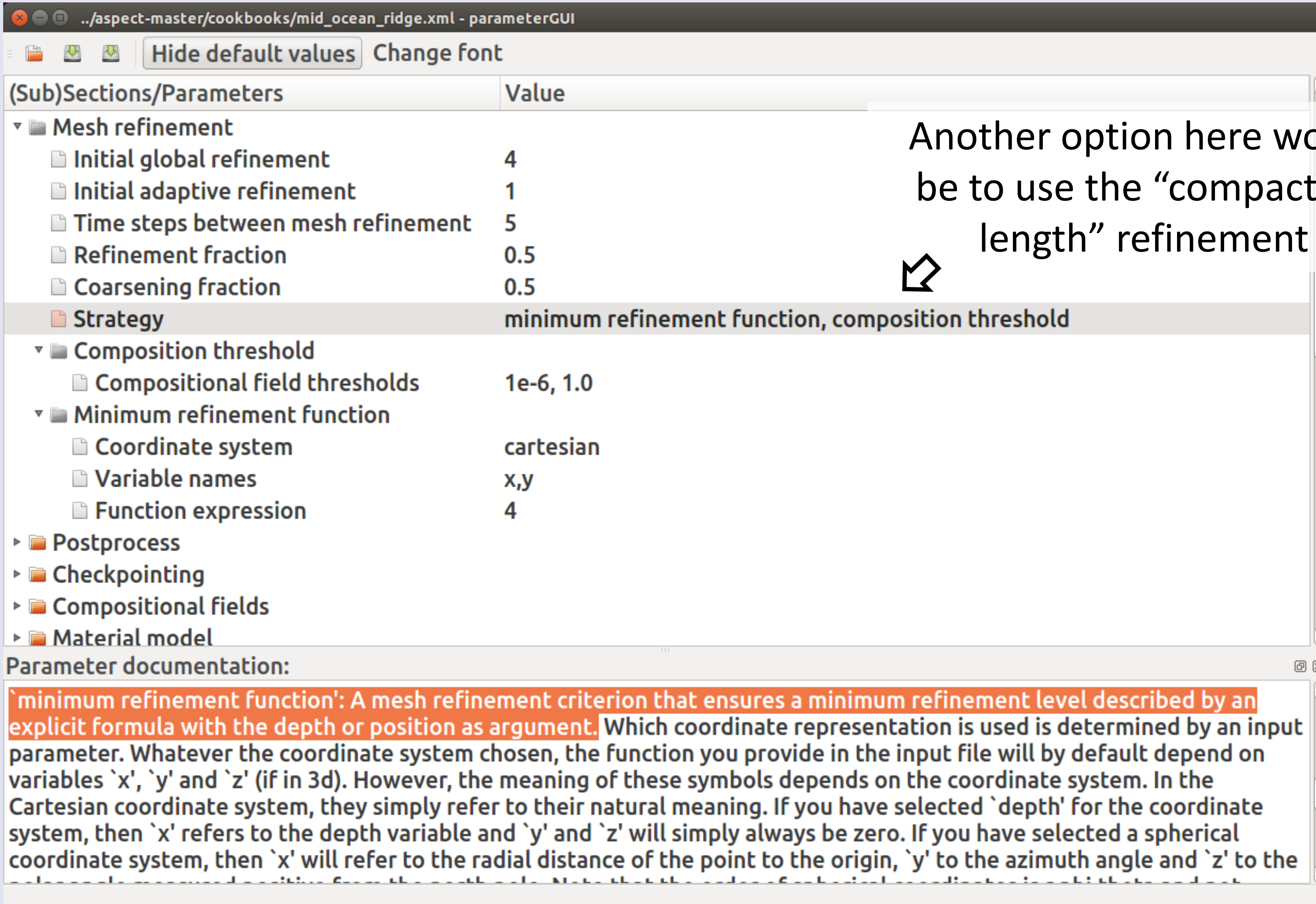
Mesh refinement

Choose the resolution based on:

The presence of melt | the compaction length



Mesh refinement



Another option here would be to use the “compaction length” refinement

Material properties

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

Melting and freezing are faster than advection

Melt is less dense than the solid

$$k_\phi = k_0 \phi^3$$

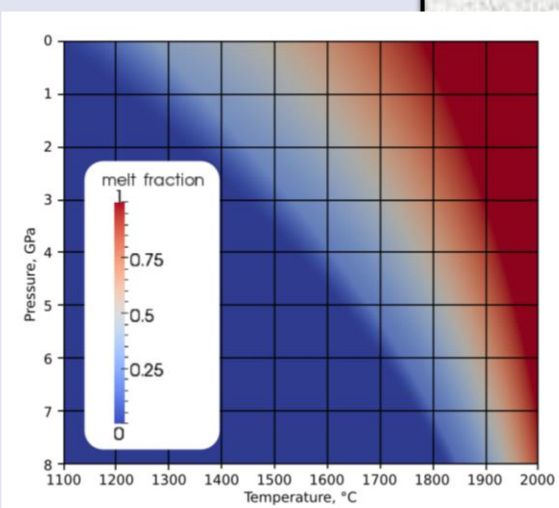
$$\eta(\phi, T) = \eta_0 e^{\alpha(\phi - \phi_0)}$$

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

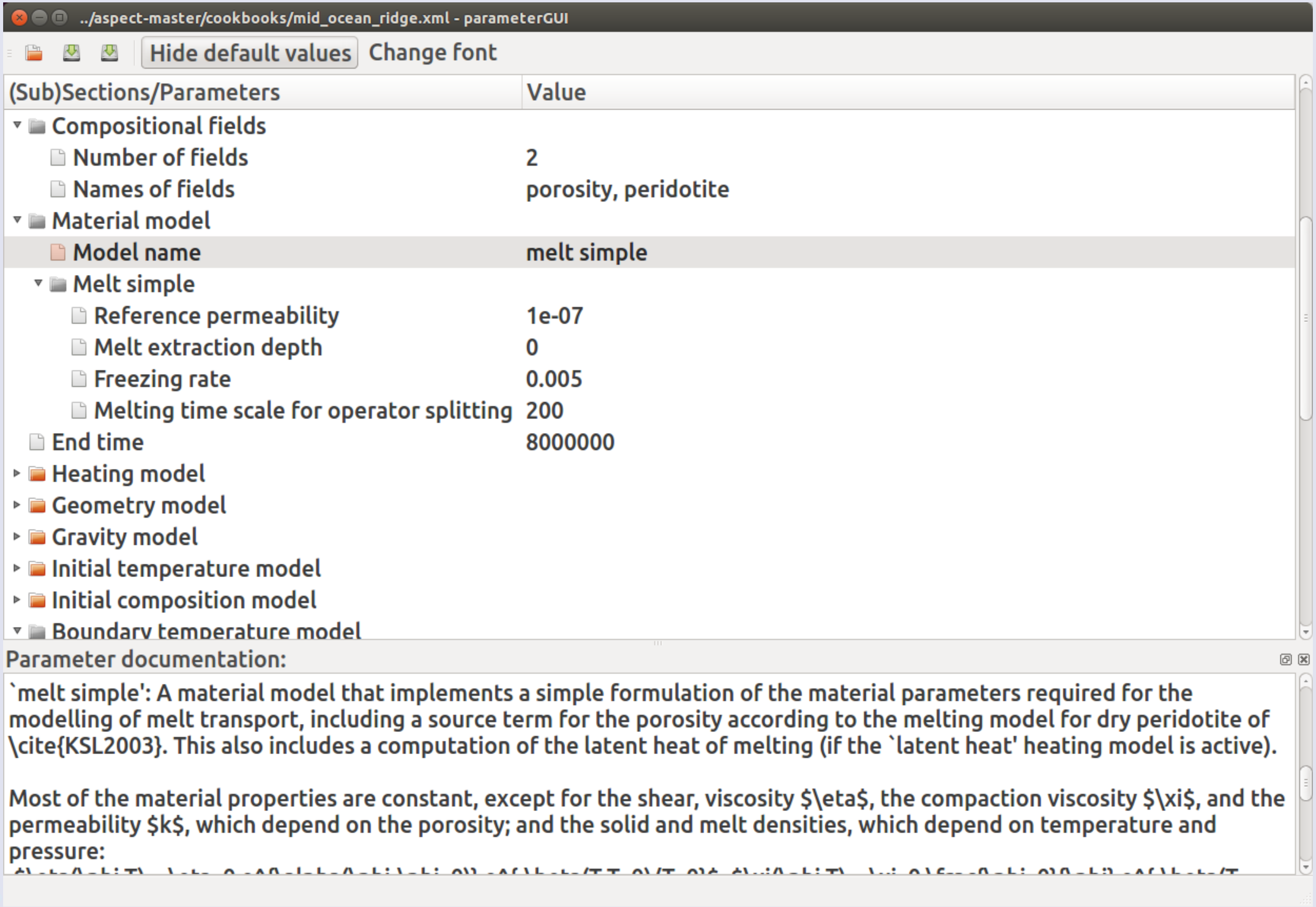
Permeability, shear and compaction viscosities depend on the porosity

Peridotite melting

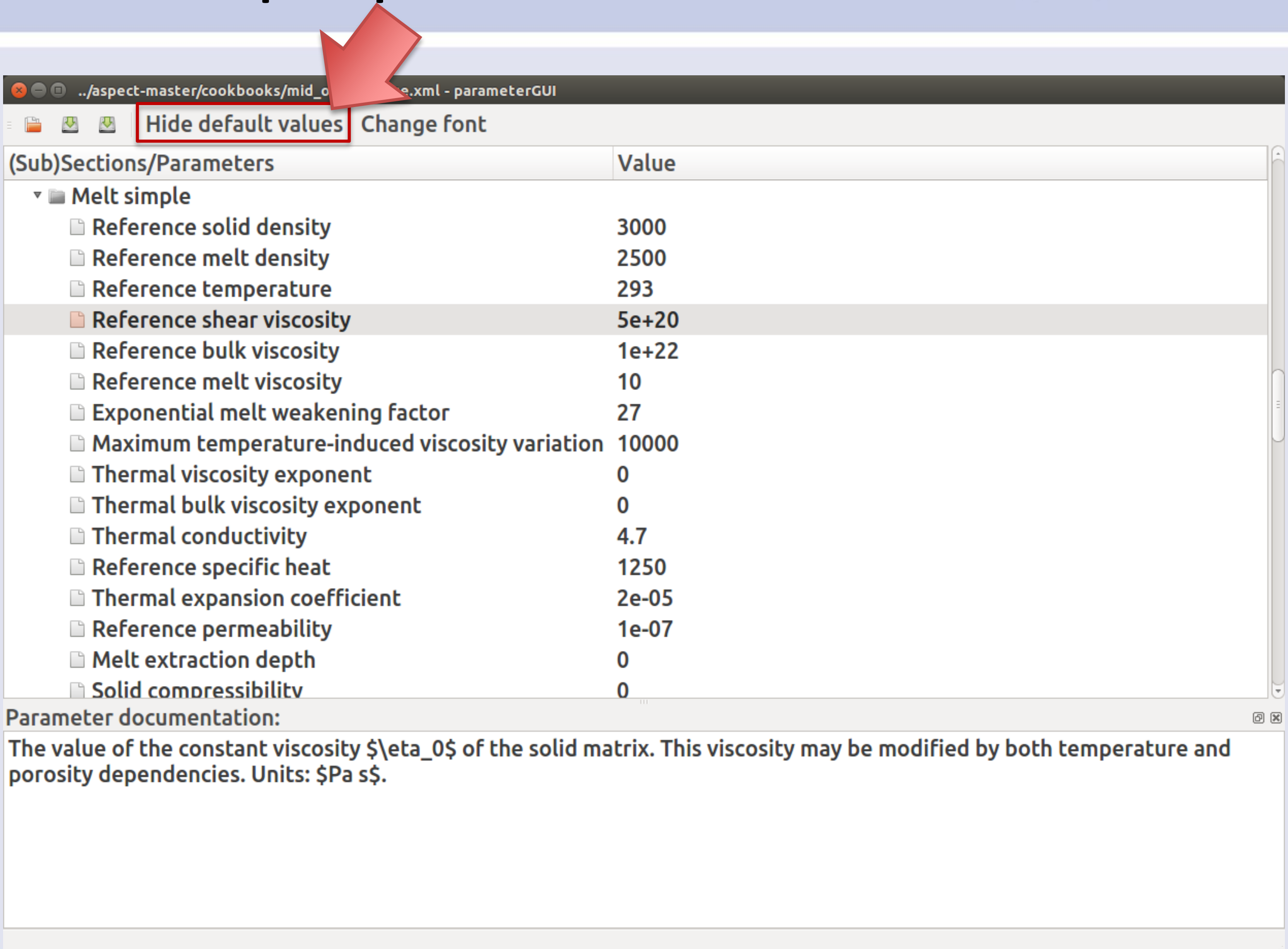
(after Katz et al., 2003)



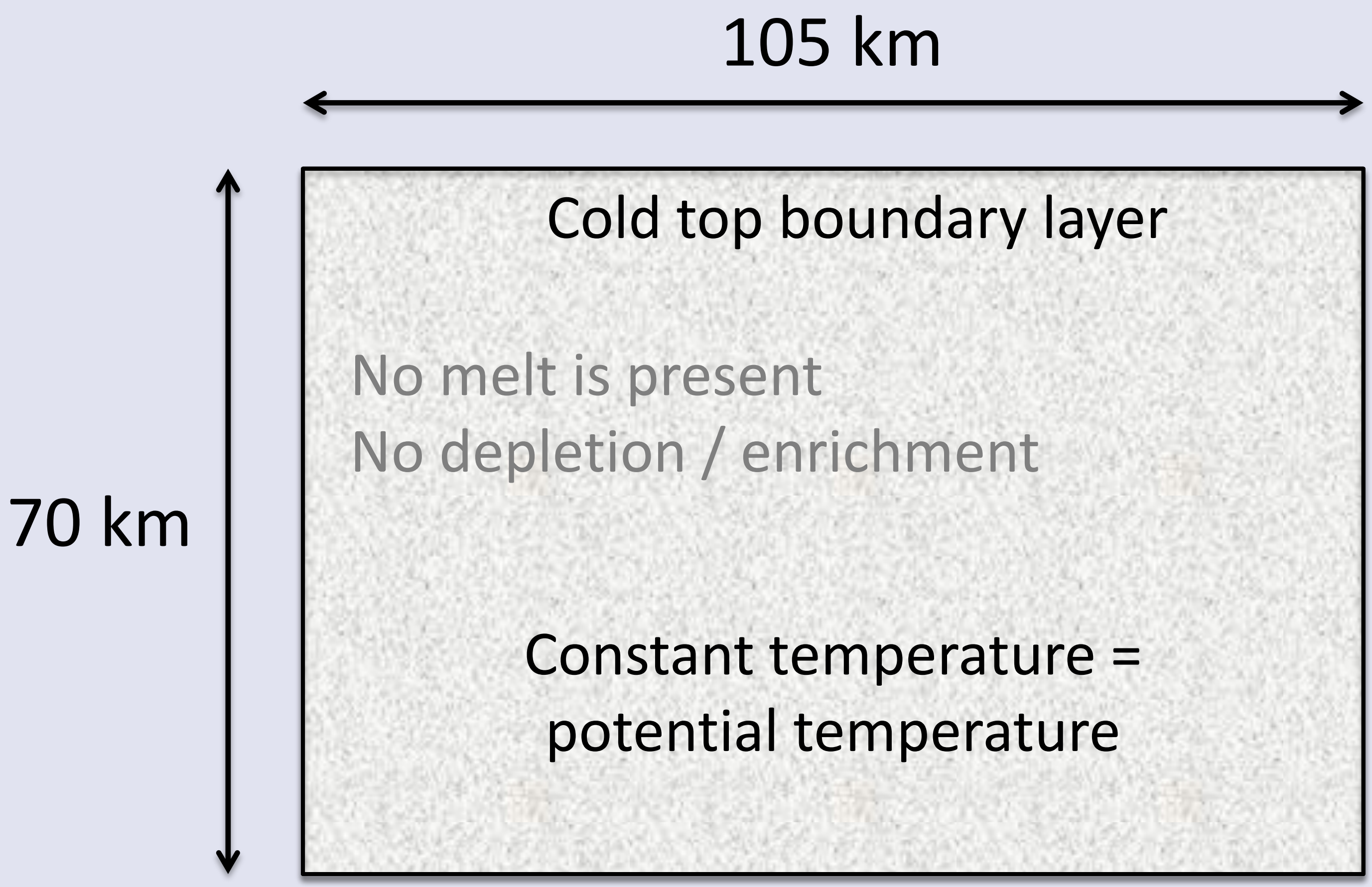
Material properties



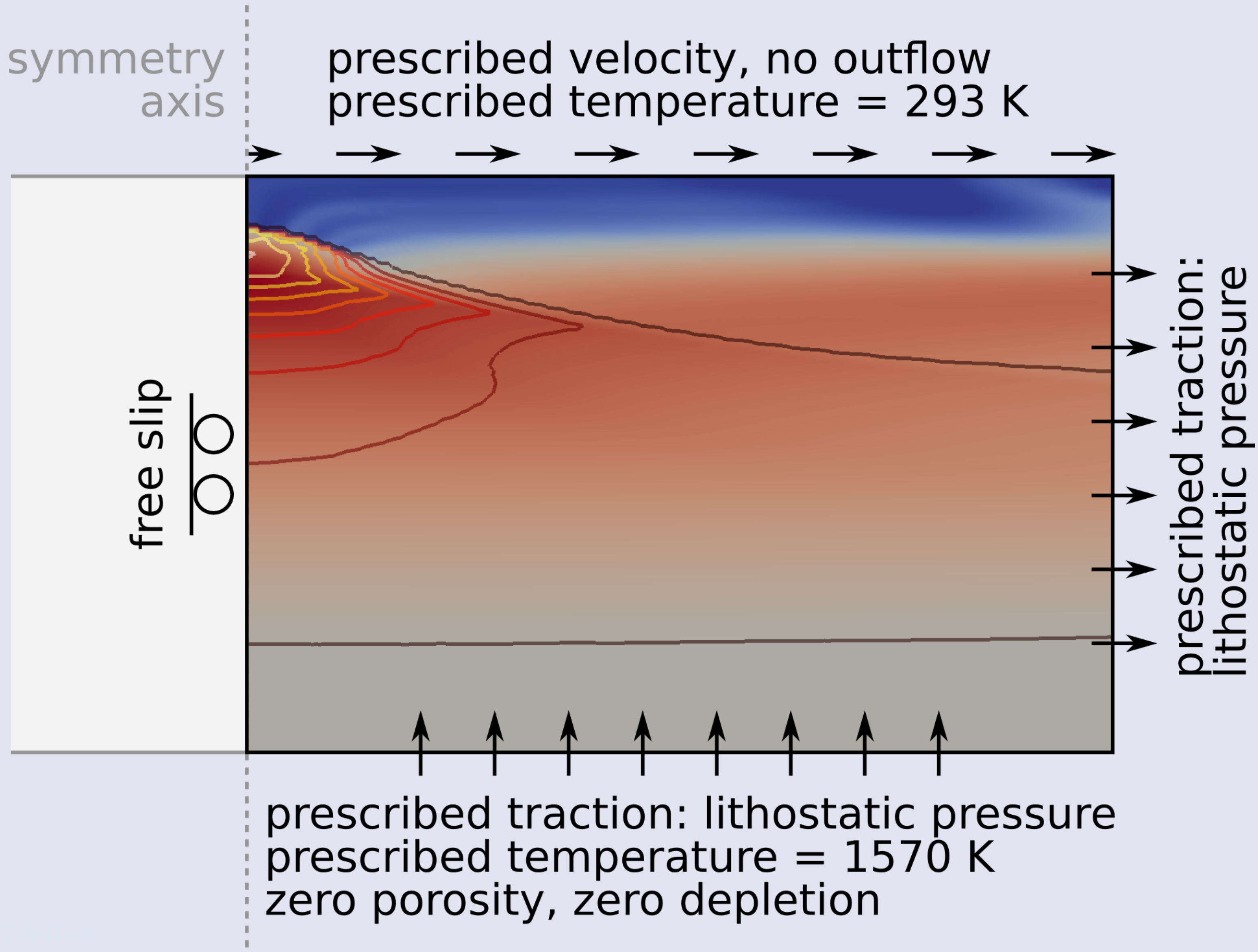
Material properties



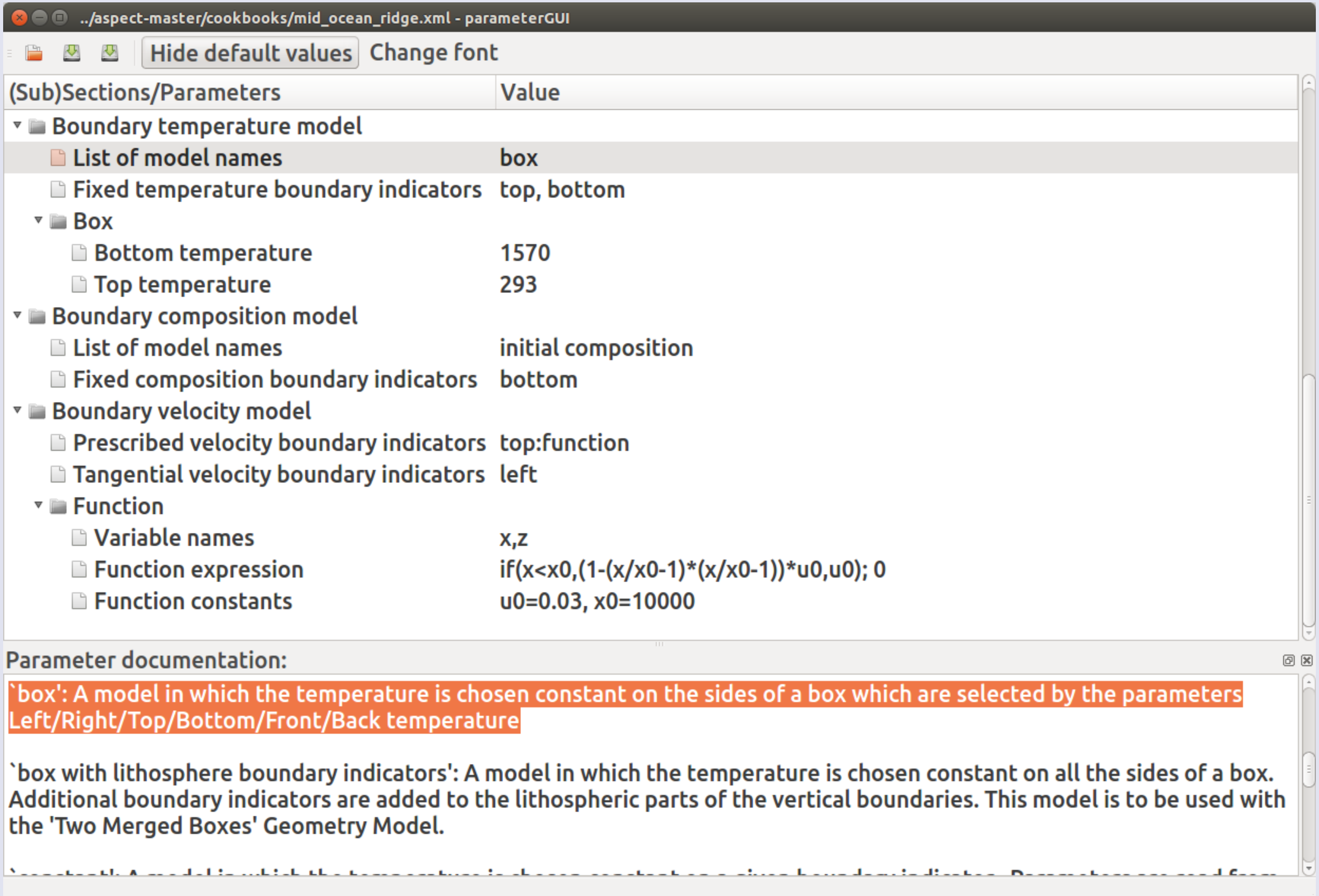
Initial conditions



Boundary conditions

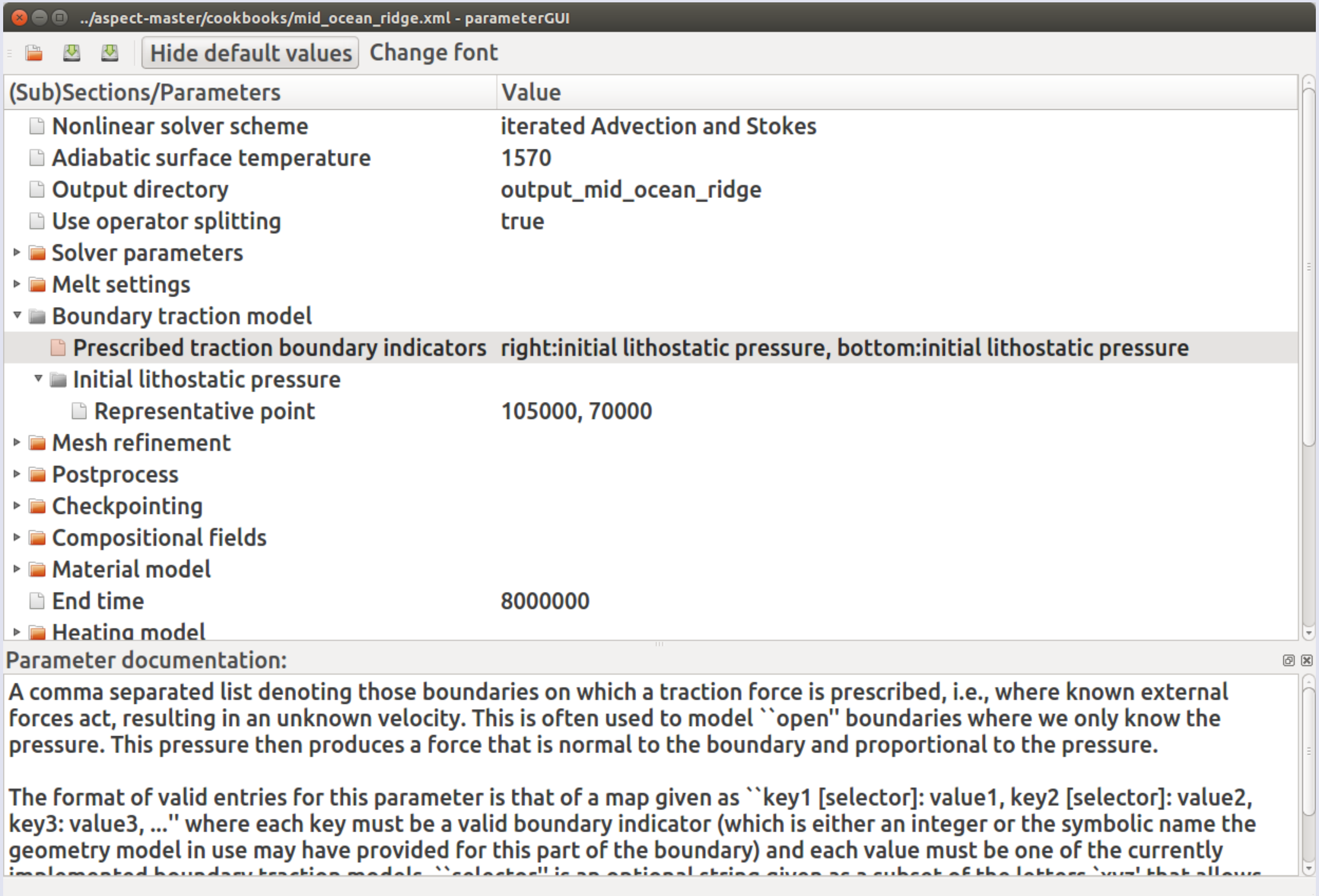


Boundary conditions

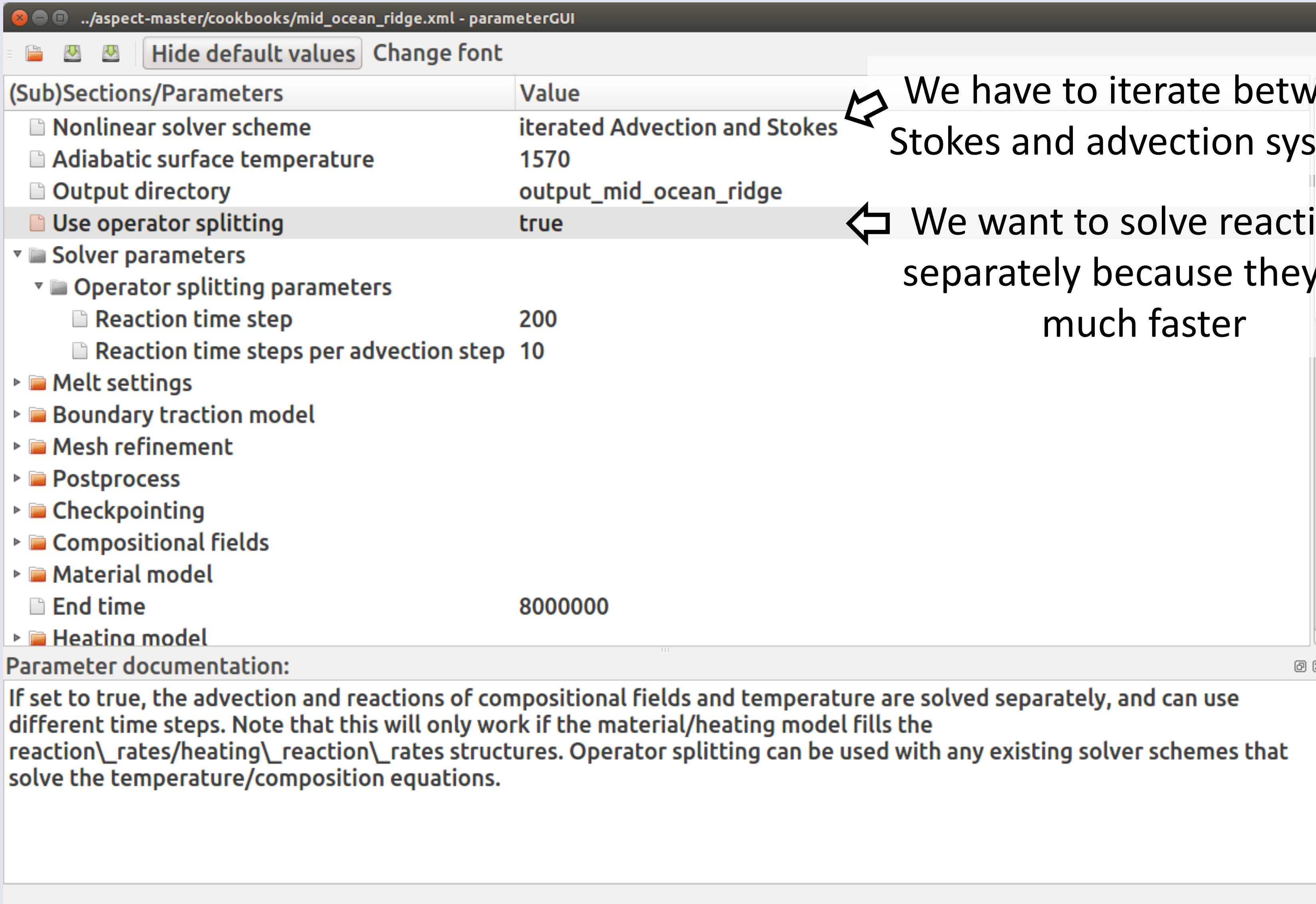


Boundary conditions

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS



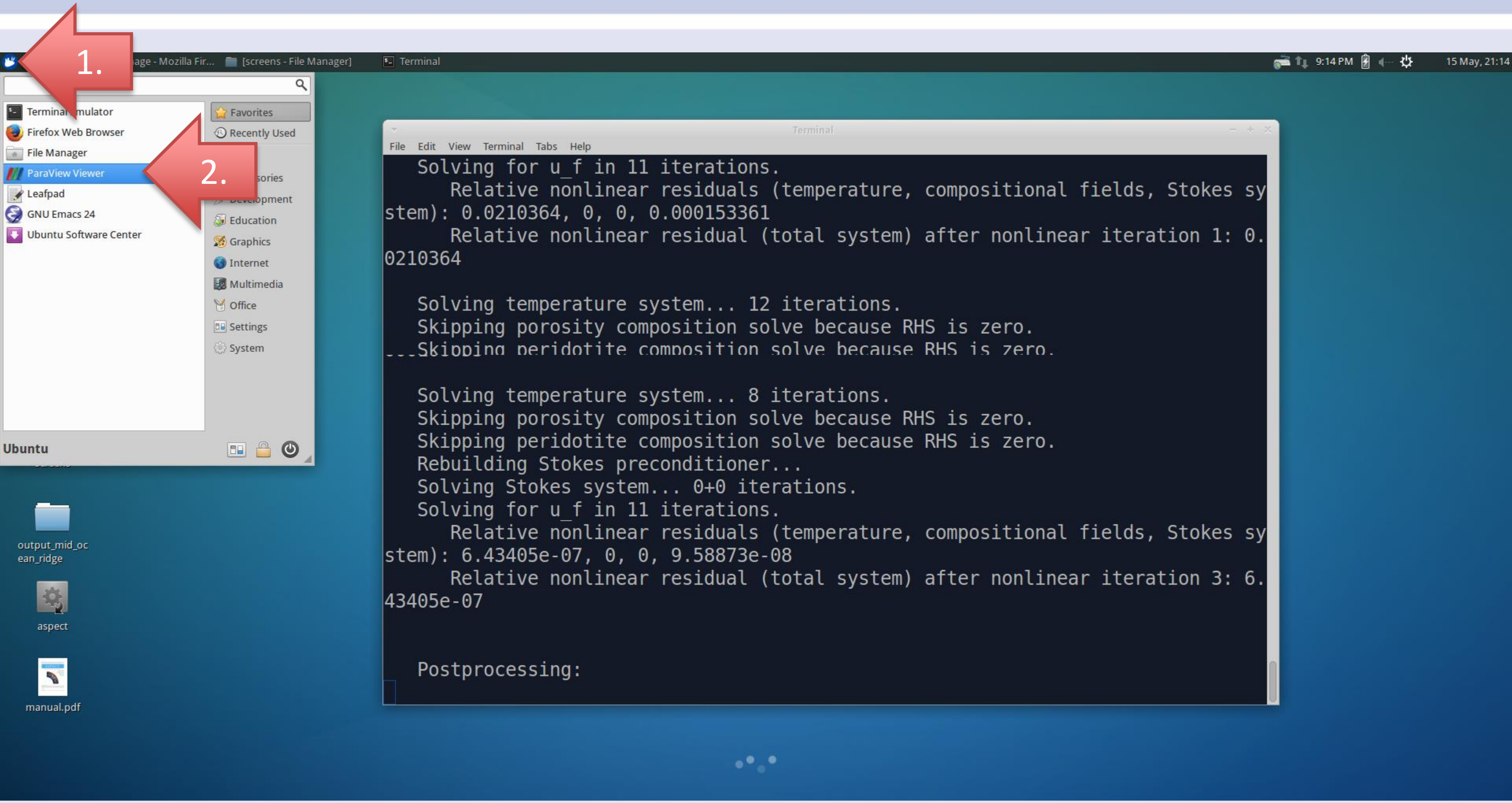
Solvers



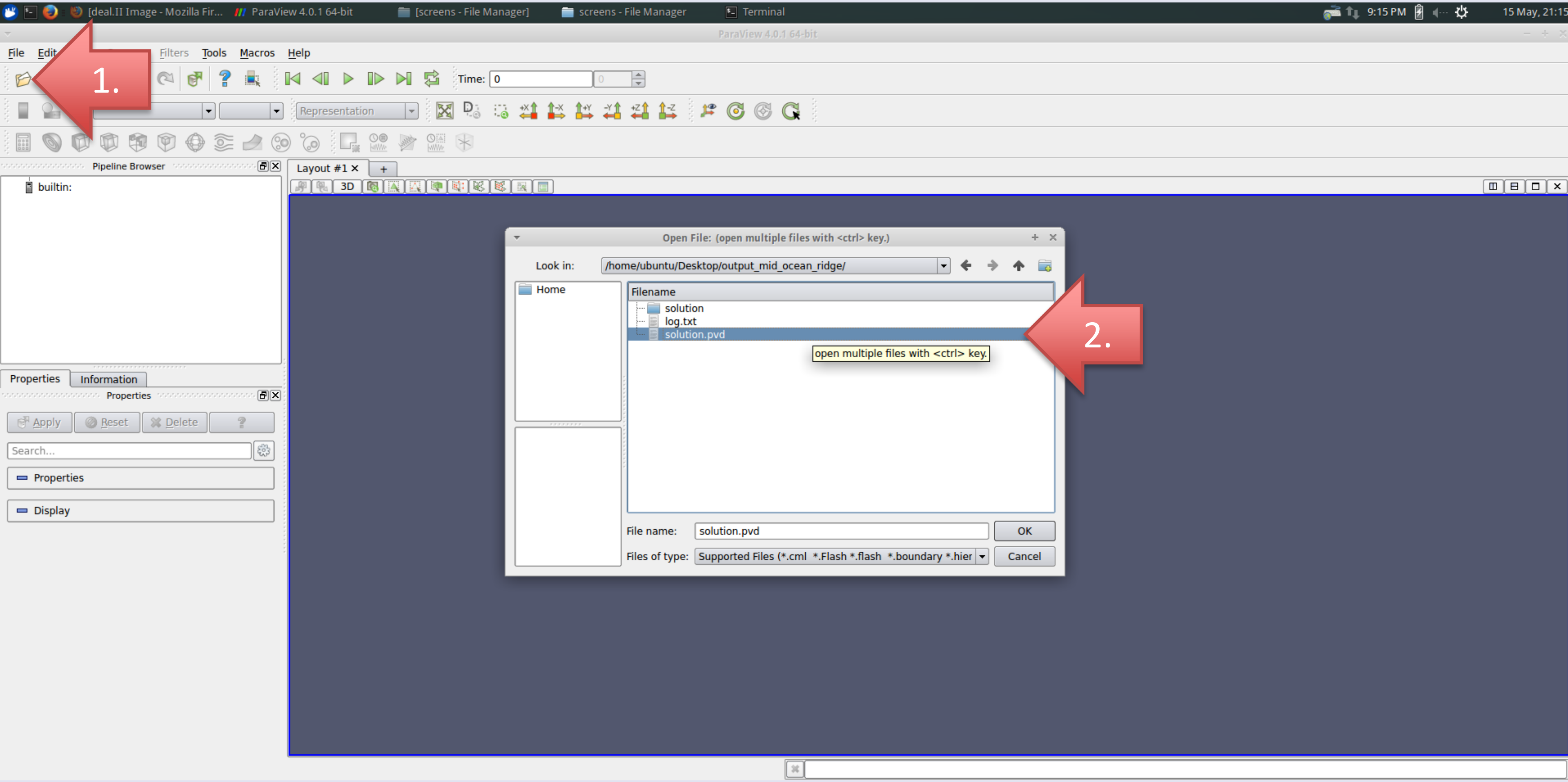
We have to iterate between Stokes and advection system!

We want to solve reactions separately because they are much faster

Paraview

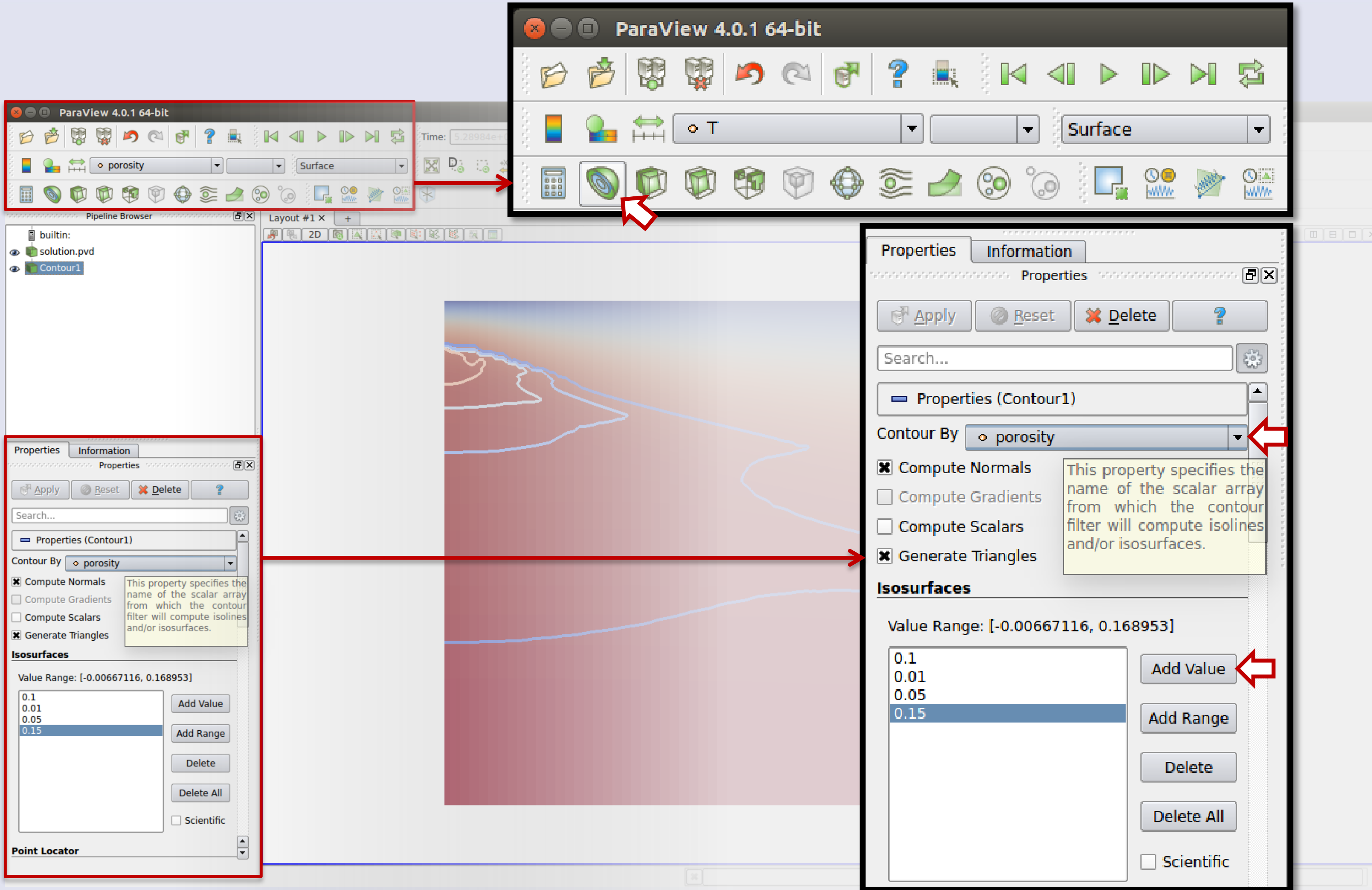

1.
2.
age - Mozilla Fir...
[screens - File Manager]
Terminal
9:14 PM
15 May, 21:14
Terminal Emulator
Firefox Web Browser
File Manager
ParaView Viewer
Leafpad
GNU Emacs 24
Ubuntu Software Center
Favorites
Recently Used
Education
Graphics
Internet
Multimedia
Office
Settings
System
Ubuntu
output_mid_ocean_ridge
aspect
manual.pdf
File Edit View Terminal Tabs Help
Solving for u_f in 11 iterations.
Relative nonlinear residuals (temperature, compositional fields, Stokes system): 0.0210364, 0, 0, 0.000153361
Relative nonlinear residual (total system) after nonlinear iteration 1: 0.0210364
Solving temperature system... 12 iterations.
Skipping porosity composition solve because RHS is zero.
Skipping peridotite composition solve because RHS is zero.
Solving temperature system... 8 iterations.
Skipping porosity composition solve because RHS is zero.
Skipping peridotite composition solve because RHS is zero.
Rebuilding Stokes preconditioner...
Solving Stokes system... 0+0 iterations.
Solving for u_f in 11 iterations.
Relative nonlinear residuals (temperature, compositional fields, Stokes system): 6.43405e-07, 0, 0, 9.58873e-08
Relative nonlinear residual (total system) after nonlinear iteration 3: 6.43405e-07
Postprocessing:

Paraview



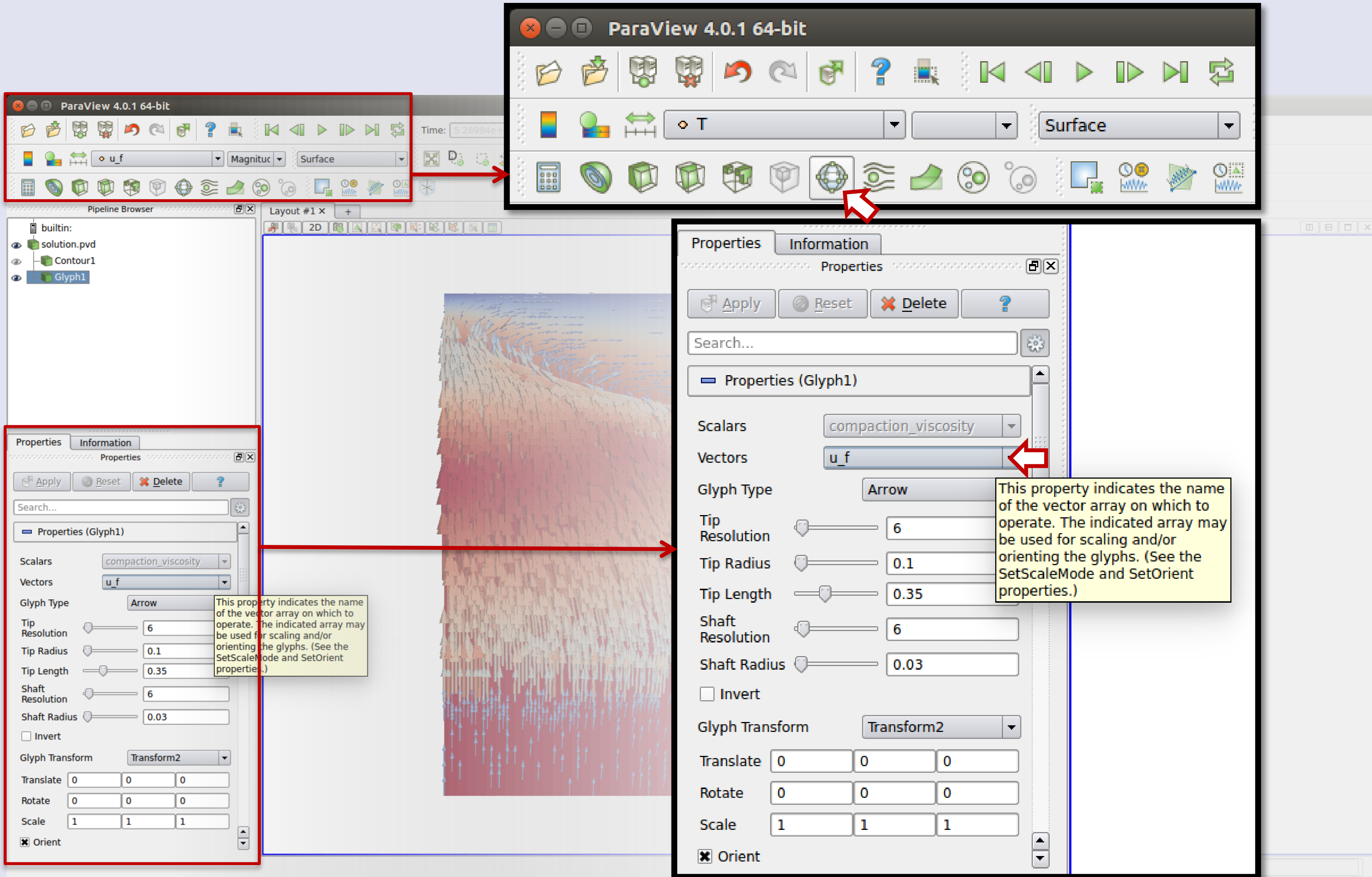
- The output file is located in: /home/ubuntu/Desktop/output_mid_ocean_ridge

Paraview: Plot contours

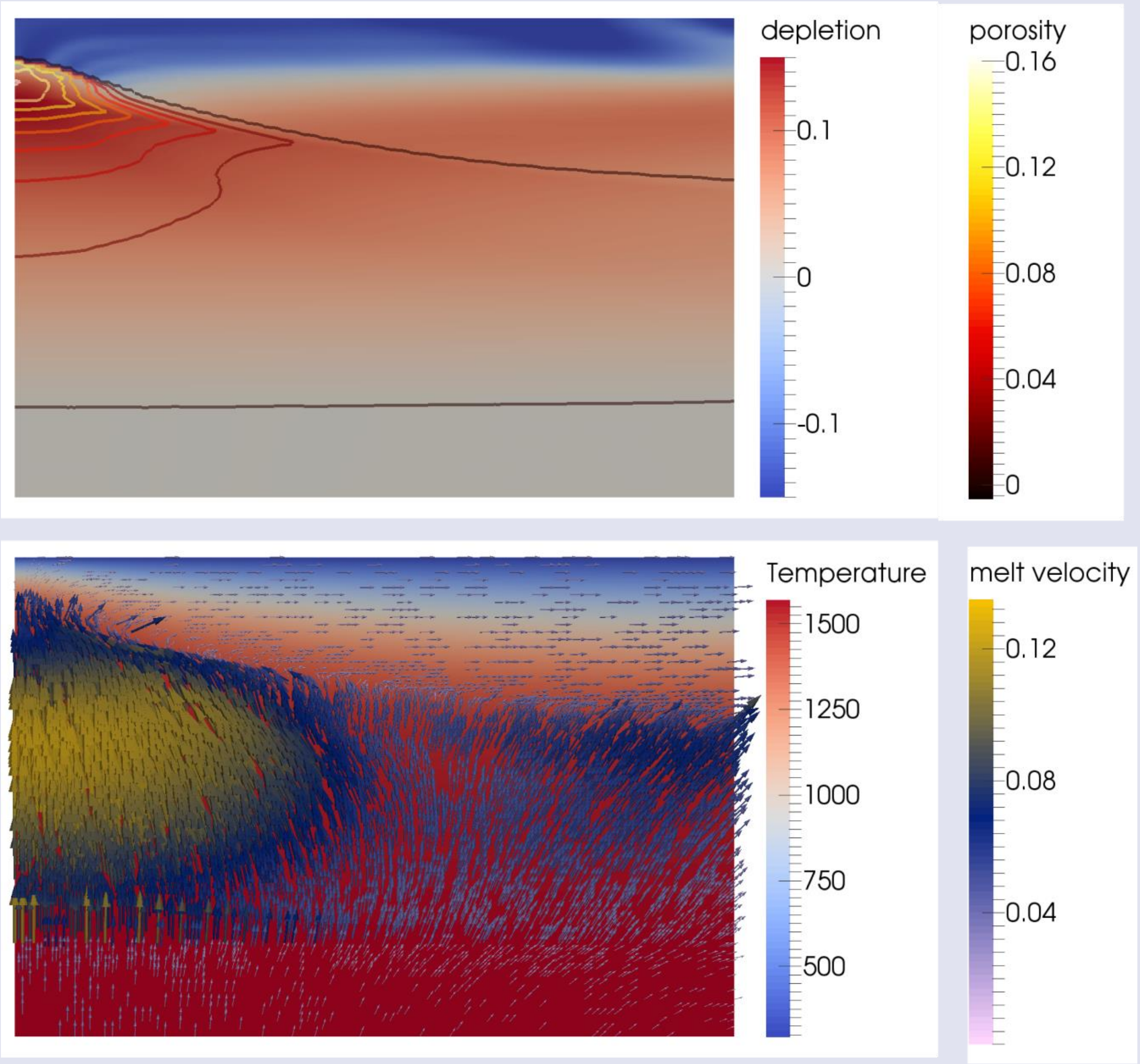


Paraview: Plot glyphs

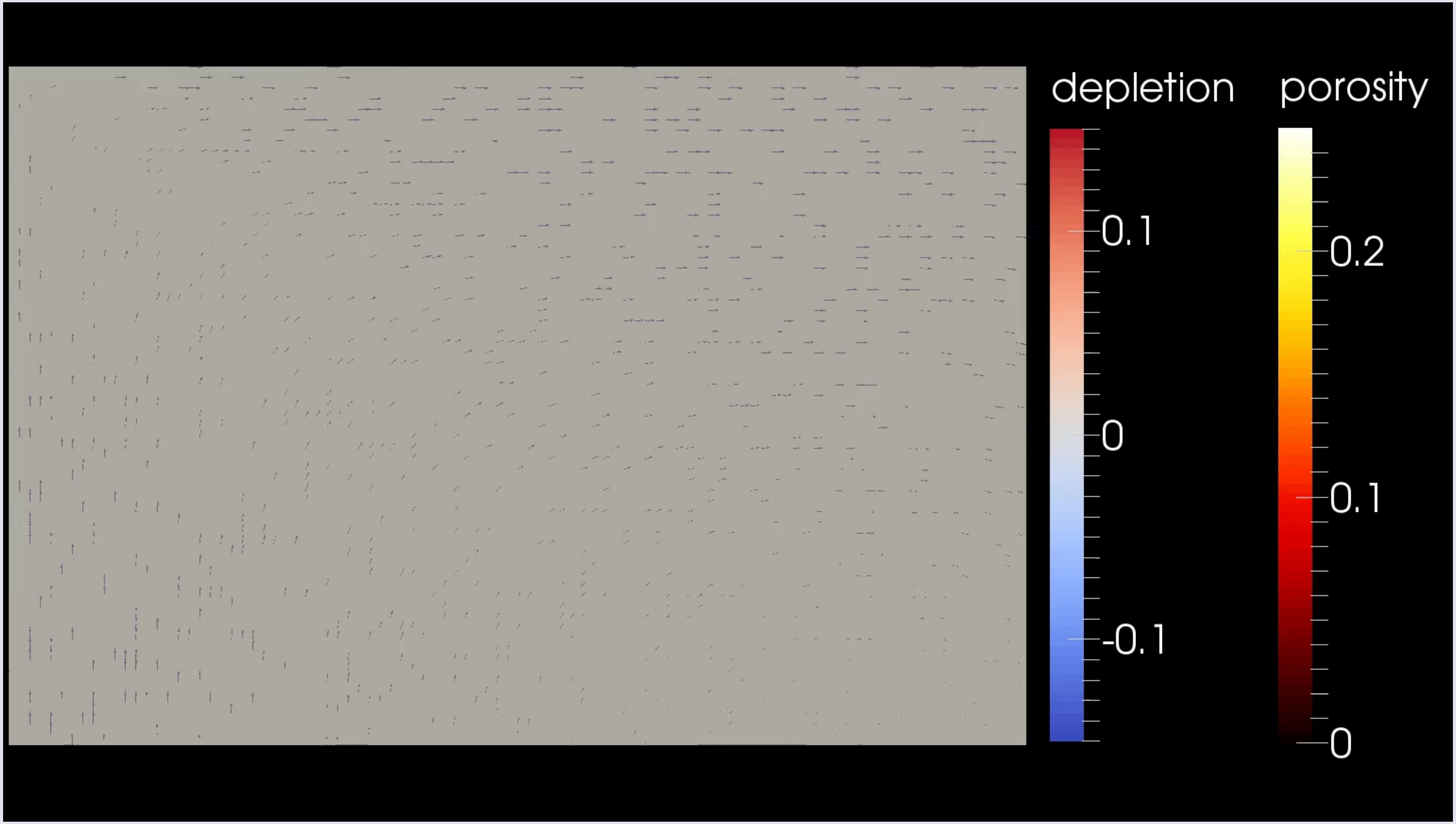
COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS



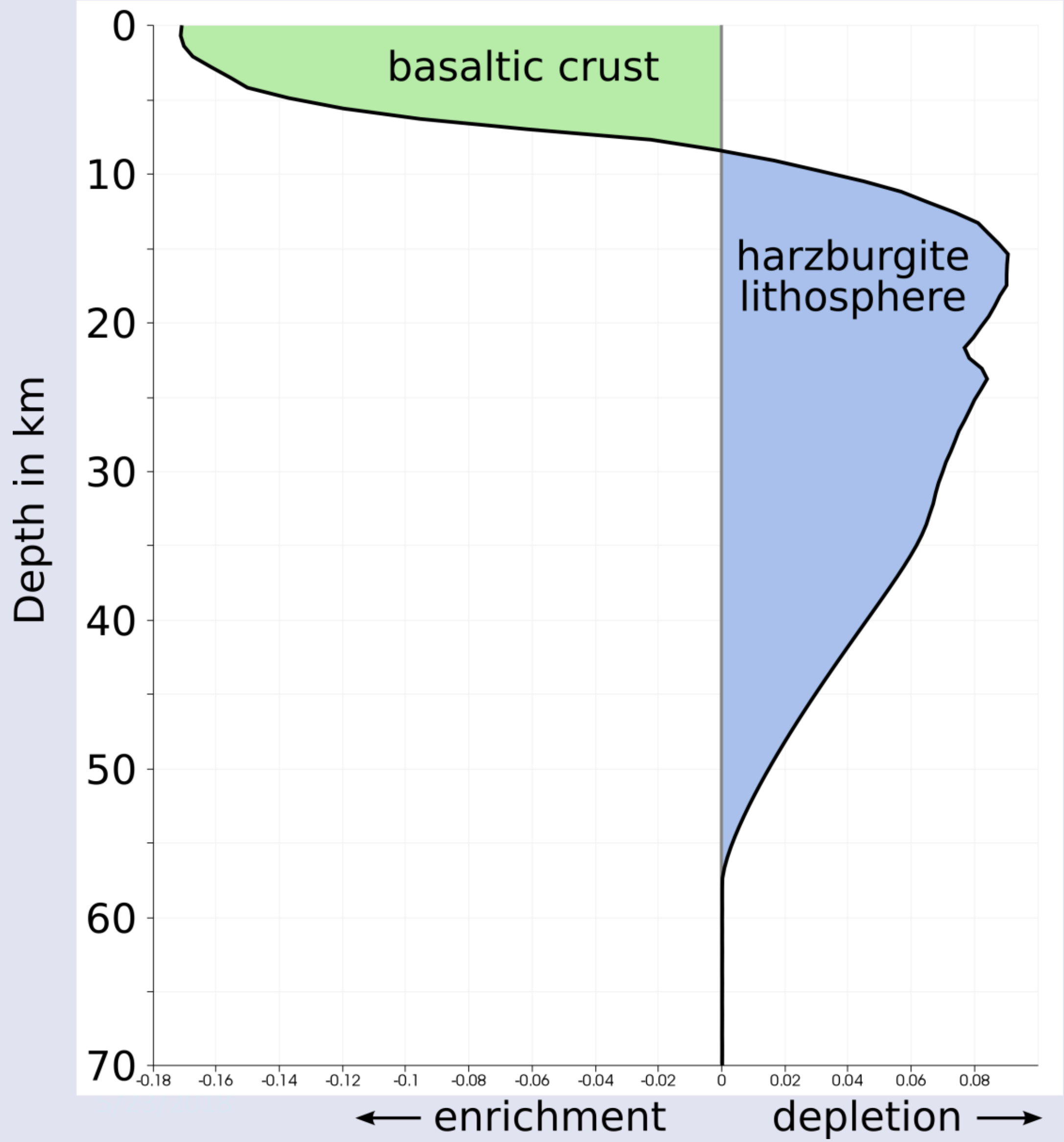
Results


depletion
0.1
0
-0.1
porosity
0.16
0.12
0.08
0.04
0
Temperature
1500
1250
1000
750
500
melt velocity
0.12
0.08
0.04

Model evolution



Results: chemical composition

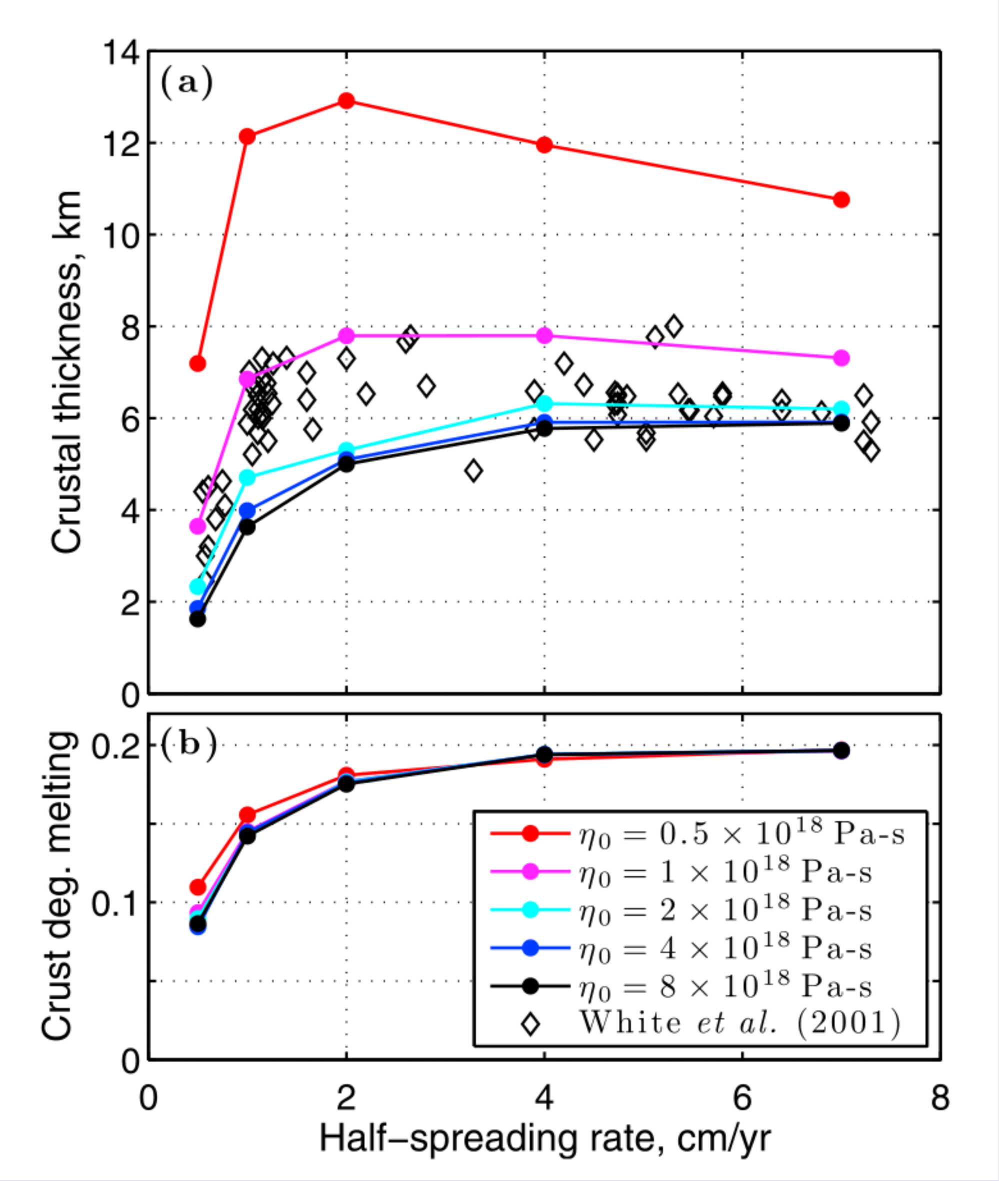


- Vertical profile though the model *(Paraview: Filters ⇨ Plot over line*
- Enriched crust
- Depleted lithosphere
- Crustal thickness: ~8 km

Things to play with

Vary:

- Spreading rate
- Shear viscosity
- Permeability
- Compaction viscosity

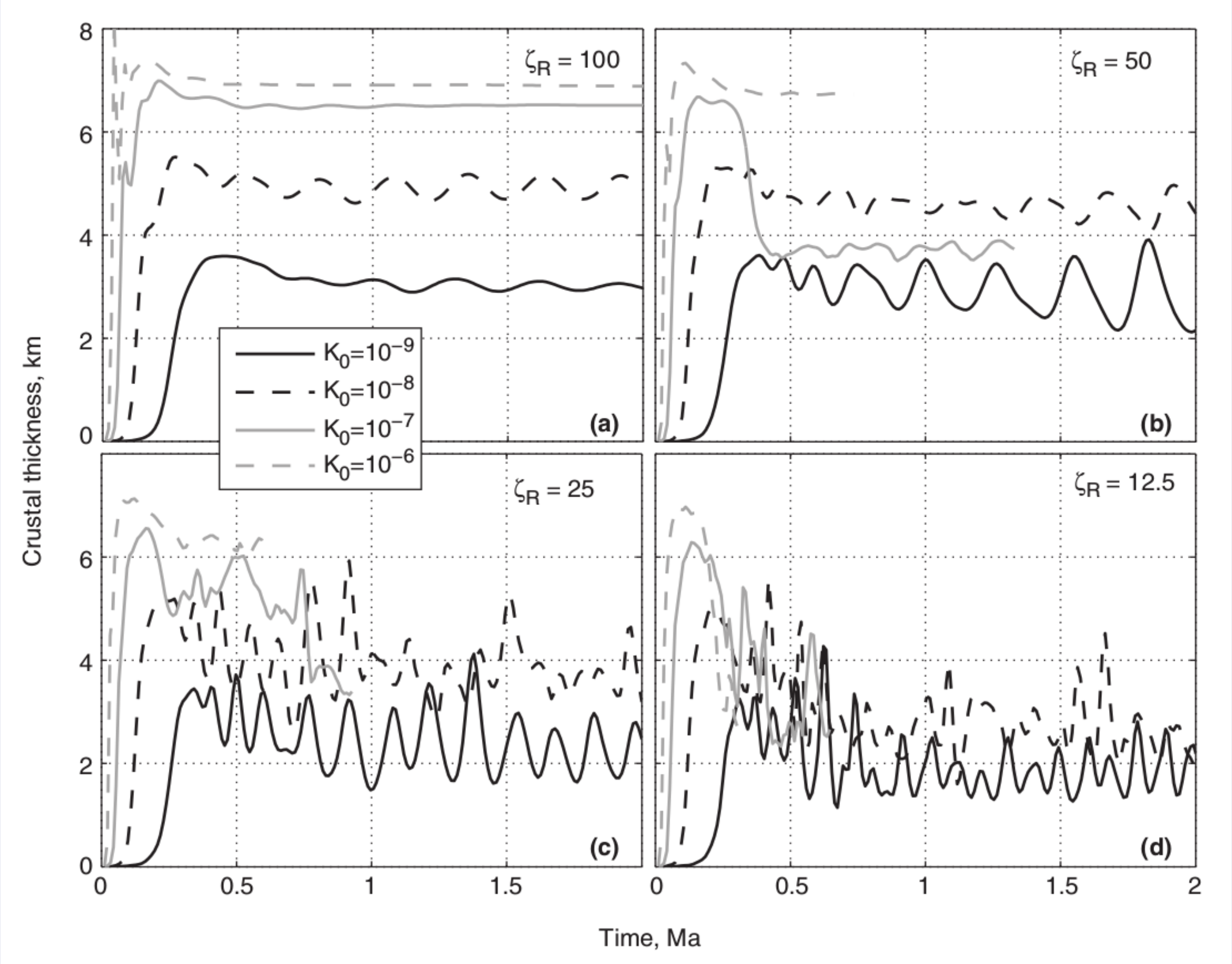


Katz, 2010

Things to play with

Vary:

- Spreading rate
- Shear viscosity
- Permeability
- Compaction viscosity



Katz, 2008

Things to play with

CIG COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

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
- Methods: Dannberg, J., & Heister, T. (2016). Compressible magma/mantle dynamics: 3-D, adaptive simulations in ASPECT. *Geophysical Journal International*, *207*(3), 1343-1366. https://doi.org/10.1093/gji/ggw329
- Ask on the mailing list: http://lists.geodynamics.org/cgi-bin/mailman/listinfo/aspect-devel