

# ASPECT HACKATHON 2015

## Bodega Bay, CA, May 19-30, 2016

### Overview

The 2015 ASPECT hackathon brought together 24 users and developers of the Advanced Solver for Problems in Earth's ConvecTion at Bodega Bay, CA. Over the course of 10 days, many features we collaboratively developed, reviewed, and merged. The hackathon also provided ample opportunity for mentoring of younger scientists by more experienced developers. The following pages list the participants and give an overview of the topics participants worked on, as well as some of the results they obtained. Most of the pictures shown and features discussed were obtained with plugins and code extensions that were merged into the main development sources of ASPECT either at the hackathon or, following more code review discussions, shortly thereafter. As shown in <https://github.com/geodynamics/aspect/graphs/contributors?from=2015-05-19&to=2015-06-30&type=c>, a total of 203 patches were merged during the hackathon and the following month, by 17 different authors. During this time, the amount of code in ASPECT grew from 75,200 to 81,100 lines. Several very large features, for example a complete rewrite of the particle code started during the hackathon by Rene Gassmoeller and Gerry Puckett and comprising several thousand lines of code, took longer than the end of June to be finished and are not included in this count.

### Participants

Anne C. Glerum	University of Utrecht, The Netherlands
Carolyn Branecky	UC Santa Cruz
Cedric Thieulot	University of Utrecht, The Netherlands
Eva Bredow	GFZ Potsdam, Germany
Gerry Puckett	UC Davis
Ian Rose	UC Berkeley
Jacky Austermann	Harvard University
Jonathan Perry-Houts	University of Oregon
Juliane Dannberg	Texas A&M University
Katrina Arredondo	UC Davis
Kimee Moore	Harvard University
Maxwell Rudolph	Portland State University
Menno Fraters	University of Utrecht, The Netherlands
Rene Gaßmüller	GFZ Potsdam, Germany
Robert Myhill	University of Bayreuth, Germany
Ryan Grove	Clemson University

Sarah Stamps	Virginia Tech
Scott Tarlow	UC Davis
Shangxin Liu	Virginia Tech
Timo Heister	Clemson University
Ying He	UC Davis
Louise Kellogg	UC Davis
Wolfgang Bangerth	Texas A&M University
Lorraine Hwang	UC Davis

## List of Projects

- Wolfgang/Timo: Review everyone's patches!
- Wolfgang: Finally get the pressure b.c. done that I started yesteryear
- Ryan: Integrating SUPG and EV with smoothing into ASPECT
- Shangxin: Comparing dynamic topography computed from higher and lower order elements; adding more tomography models as initial conditions; fixing manual typos.
- Juliane: Melt transport and helping other people
- Timo: BA, TALA, etc. as an easy to set option
- Jacky: Benchmark and cookbook with S40RTS (global convection model, dynamic topography); geoid
- Cedric: Spoint model (visco-plastic model + AMR + free surface + large deformation), N-sinker problem.
- Rene: Tracer/particle structure, geoid pp, Cell reference and velocity in material model
- Bob:
  - New material models
    - extensible [see Ian]
    - generic diffusion-dislocation creep (DONE)
    - including Peierls [implemented, currently slow to converge]
  - add global constants (average g, R etc. etc.) and strip from material models
  - benchmarks for reaction-driven overpressure (not possible in ASPECT)
  - free surface for lower boundary? [see Ian]
  - create cookbook for subduction w/ ascii data, diff\_disl
  - create chunk geometry model (DONE)
  - update spherical\_shell conditions to take chunk geometry information (DONE)
  - Still to do:
    - Periodic boundary conditions for longitude for chunk geometry (NEEDS UPDATE TO deal.ii)
    - create TerselInterface (waiting for depends to be removed)
- Jonathan: prescribed internal velocity, anisotropic viscosity, melt transport???, update material models to newer interface

- Carolyn: pressure boundary conditions, nonlinear rheology, initial lithospheric geometries
- Scott: Internal velocity boundary conditions, Lattice Preferred Orientation calculations, also interested in tracer/particles and complex viscosity structures.
- Ying He: writing codes for an monotone temperature equation using Local Discontinuous Galerkin Element method. Comparing the results with the code using continuous FEM method.
- Sarah: updated ASPECT installation instructions for TACC Stampede supercluster, extend stress postprocessor to output tractions at user-specified locations
- Anne:
  - a. Add boundary selectors (xyz) to Wolfgang's prescribed traction boundary conditions
  - b. Write plugin to calculate lithospheric pressure based on initial temperature and composition conditions for prescribed traction boundary conditions
  - c. Cookbook with Carolyn on using pressure boundary conditions to model ice sheet loading
  - d. Simple plastic material model.
  - e. iterated\_Stokes solver: use same initial Stokes residual as iterated\_IMPES
  - f. iterated\_IMPES: rebuild preconditioners every nonlinear iteration
  - g. Improve on initial composition plugin for instantaneous dynamics subduction model.
  - h. Geometry model with additional boundary indicators for vertical sides of lithosphere
  - i. Principal stress axes postprocessor?
  - j. Different nonlinear tolerance/max nr of nonlinear iterations during t0/prerefinement steps/late timesteps
- Ian : free surface stuff, geoid, benchmarks, composable material models
- Ian : is there interest in a GMT plugin? Yes - scott (Max and Bob too)
- Max: Verify that periodic boundary conditions (in 2D cartesian geometry) now work at high Ra. Geoid. Depth-averaged quantities. Cookbook with mixed free-slip/prescribed velocity boundary conditions at surface.
  - a.
- Eva: adjust the style of the Gplates Plugin to that of the Ascii Data Plugin and make it applicable for box geometries
- Louise: Cookbook and benchmark - spherical convection
- Gerry: Implement and / or debug passive tracer particles in the following cases
  1. Correctly implement the various particle integration algorithms:
    - i. Euler
    - ii. Second-order Runge-Kutta
    - iii. Fourth-order Runge-Kutta

The high-order Runge-Kutta methods require the velocity at the particle positions at intermediate times, i.e., times between timesteps, which will require interpolation in time.

    - a. Done! For for Euler and RK2.

- b. RK4 is coded, but needs to be tested. RK4 also needs to be checked to see if it is fourth-order accurate.
- 2. Debug the loss of particles or misplacement of particles when one runs ASPECT on more than one processor: This is due to non unique particle ids, which are used in the second-order and fourth-order Runge-Kutta integrators, but not in the first-order Euler integrator.
  - Done! For Euler and RK2.
- 3. Implement a 2D circular Stokes flow field and test to determine if the convergence rates of Euler, second-order Runge-Kutta and fourth-order Runge-Kutta equal their design (i.e., theoretical) convergence rates.
- 4. Implement a post-processor to compute the convergence rate of the various particle integration algorithms:
  - i. Euler
  - ii. Second-order Runge-Kutta
  - iii. Fourth-order Runge-Kutta
 and create a Tracer Particle Test.

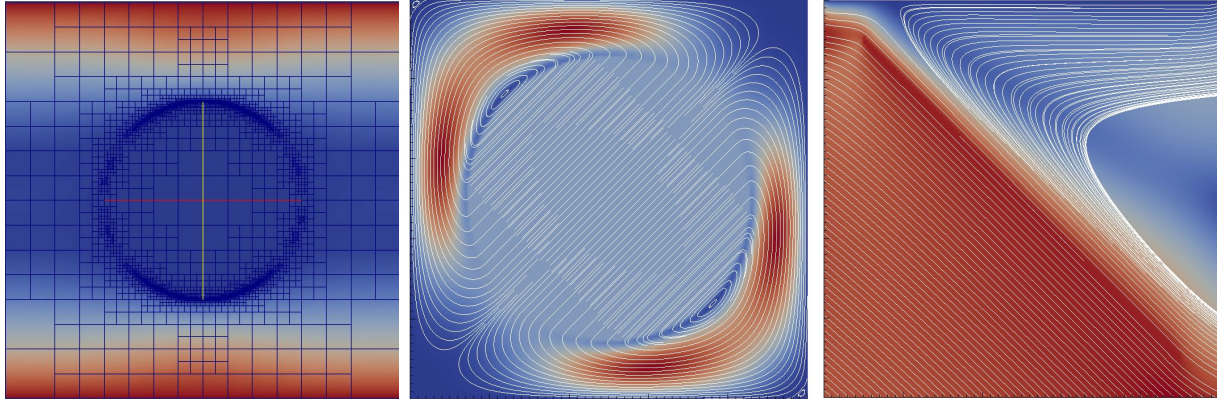
Implementing this the way Timo suggested I do it requires accessing the Particle World from the post-processor in order to obtain the initial and final particle positions.

- 5. Merge the appropriate parts of
  - i. Rene's van-keken-smooth-tracer.prm with tests/prescribed\_stokes\_solution.prm
    - Done! The new parameter file is called circular\_tracer\_flow.prm.
  - ii. Check the convergence rates as a function of dt.
    - In progress on Friday, May 29, 2015 at 11:48:54 PDT.

- Menno: Add weighted version of averages to material averaging
- Menno: Add plugin to be able to control the minimum and maximum refinement level based on model values such as temperature, density, etc..
- Menno: Work on ellipsoid geometry model
- Kimee: extend latent-heat mode to allow for option of phase changes defined by pressure and temperature, instead of depth and temperature
- Kimee: edited error messages
- Kimee: deleted x\_depends\_on() functions in code, replaced with updated dependence structure all throughout code.

## An overview of completed projects

### Johnathan Perry-Houts

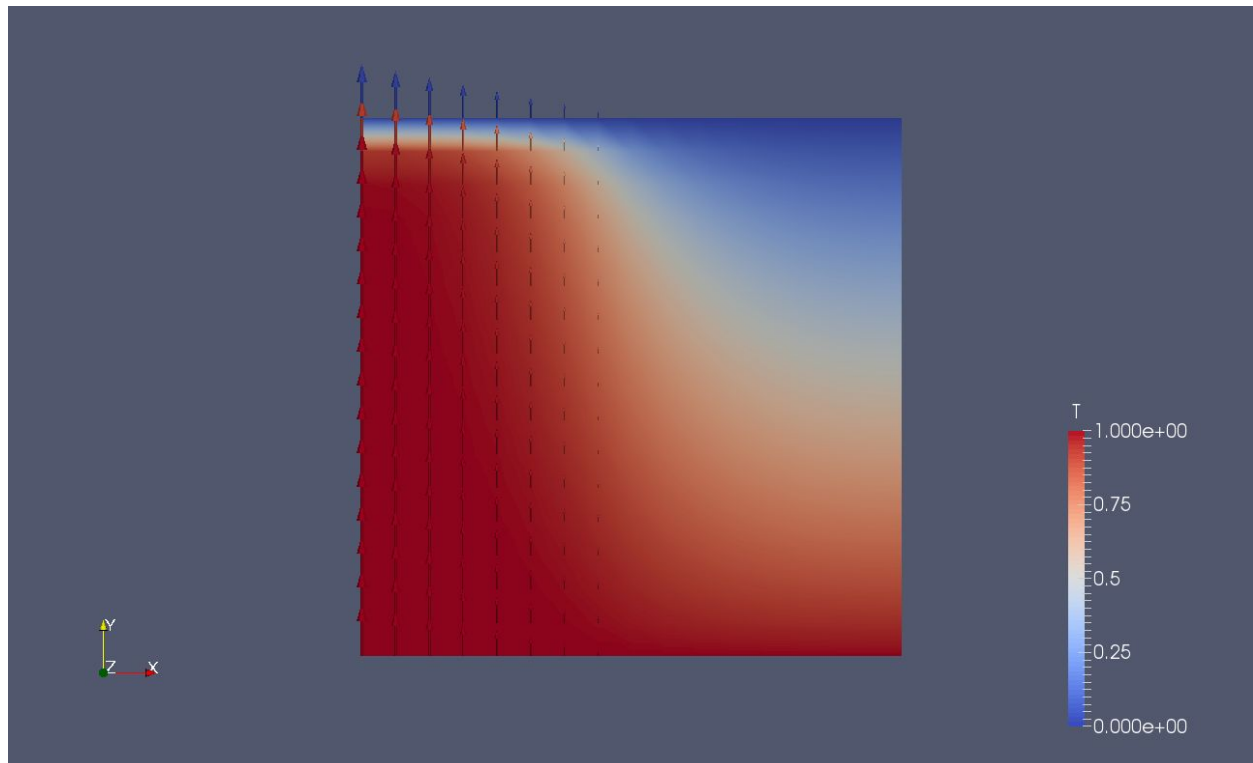


Some examples of prescribed internal velocities (in only selected cells, with Stokes solved on all other cells). A description of how to do this is included in the manual as a new cookbook, and working examples included in `/cookbooks/prescribed_velocity/` directory.

I also updated the Simple material model, from which many other models inherit, to the new(ish) interface rather than the compatibility interface. This included fixes to several bugs which were uncovered in the process.

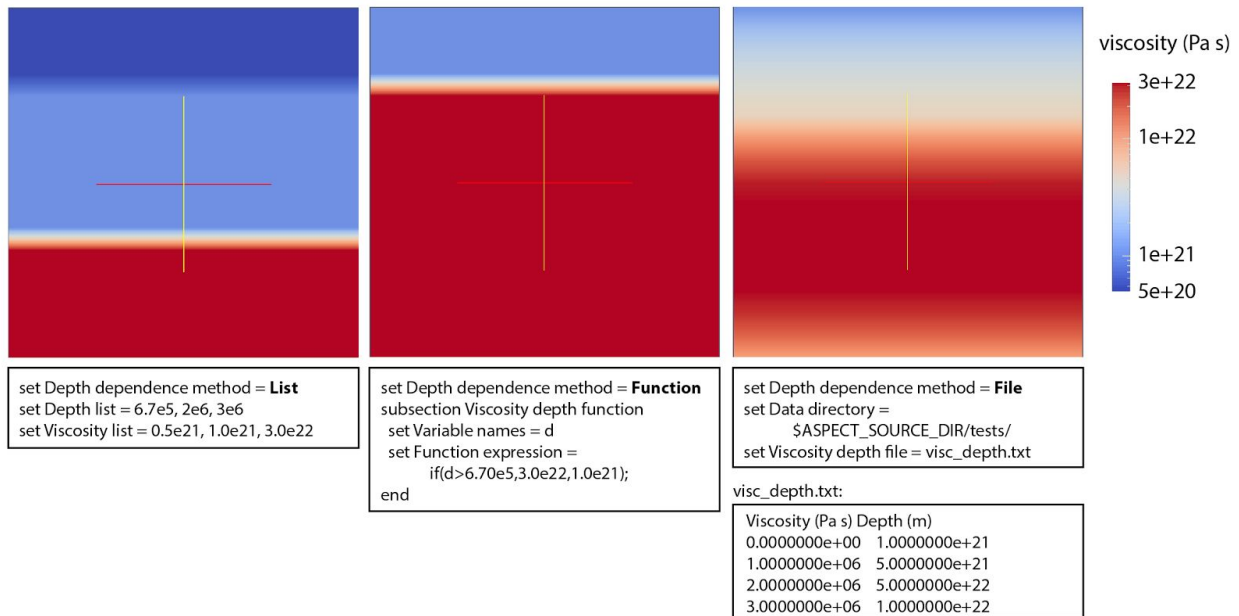
Made some progress towards an implementation of anisotropic viscosity.

## Scott Tarlow



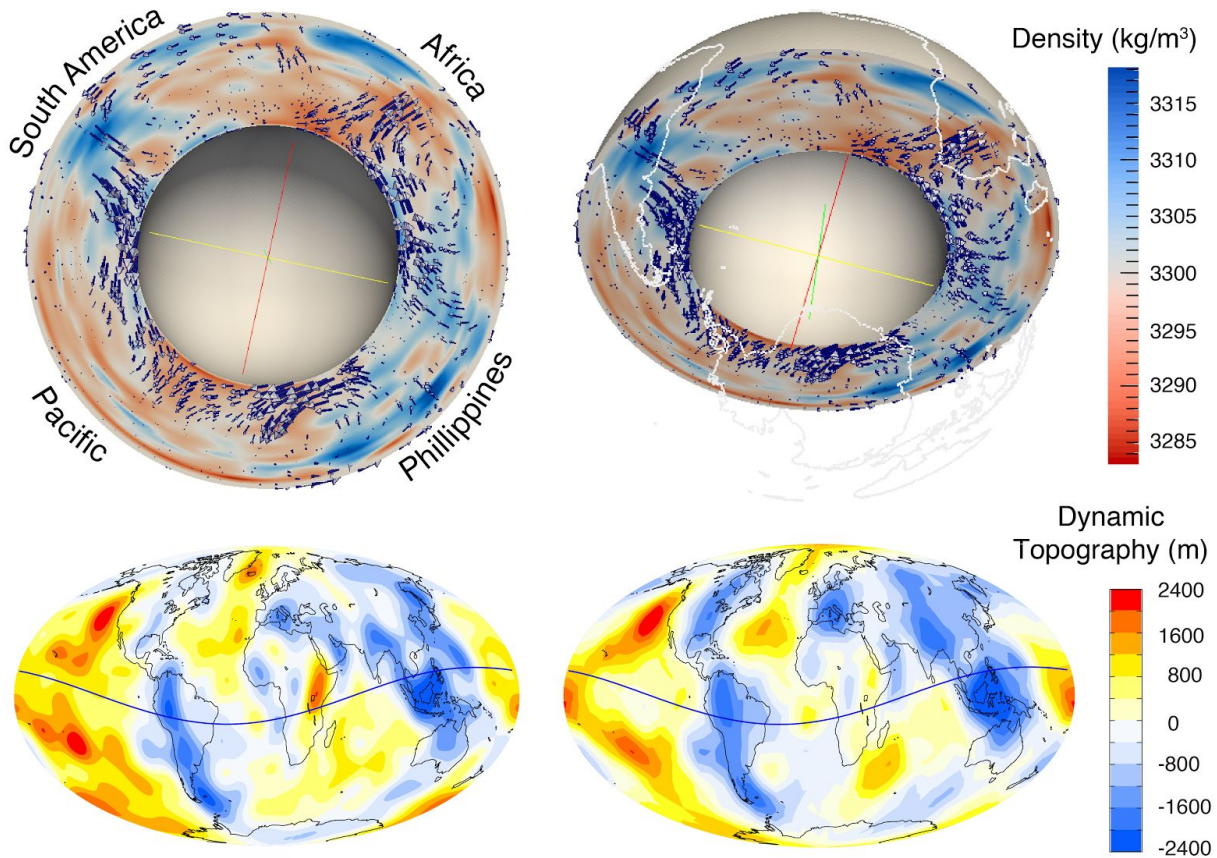
Above is a velocity field prescribed by an ascii file. In this method, the Stokes flow is turned off, allowing the user to prescribe the velocities at any point in the mesh. As you can see the velocity field decreases in the positive x direction until 0.

## Max Rudolph and Jacky Austermann



We included a new material model (depth\_dependent.cc) that assigns depth dependent viscosity. For this model one chooses a base model for all the other parameters (e.g. simple) and then a method for the depth dependence of viscosity. The three options are 'List' (layered viscosity), 'Function' (depth variation according to the provided function), and 'File' (read in viscosity from file and interpolate linearly). Three examples (for the three methods) are shown in the figure above. The default method if nothing is prescribed chooses the viscosity of the base model.

## Jacky Austermann



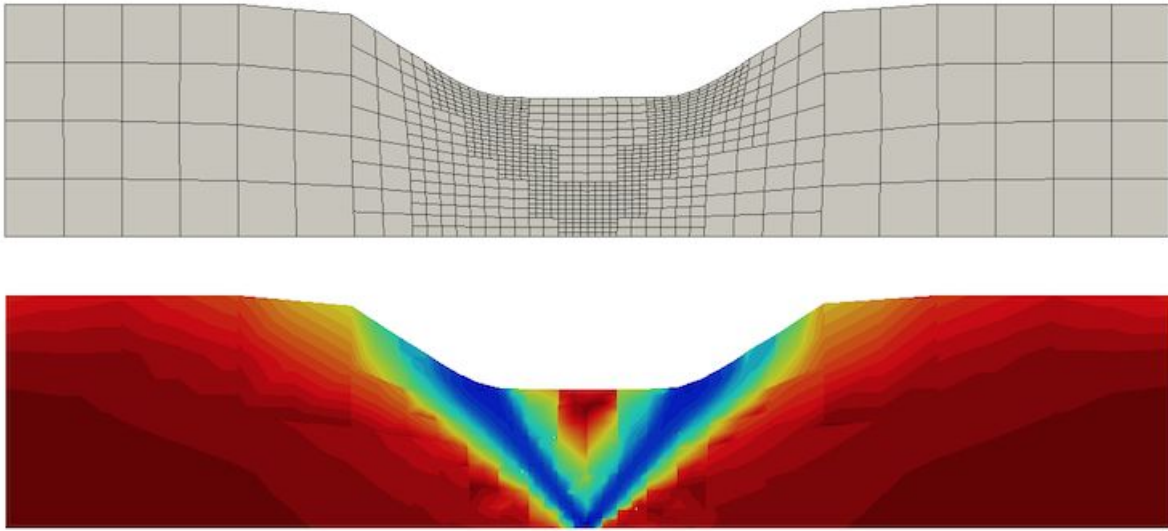
I wrote an initial condition cookbook for the manual, which takes shear wave velocity perturbations from S20RTS and maps them into density perturbations. This causes mantle convection as shown by the velocity arrows in the upper panels. The calculated flow field can be used to determine dynamic topography at the surface, which is shown in the bottom row. The left figure is based on a run with a global refinement of 4, while the right figure is based on a global refinement of 2.

## Cedric Thieulot

I worked this week on two cookbooks and a plugin.

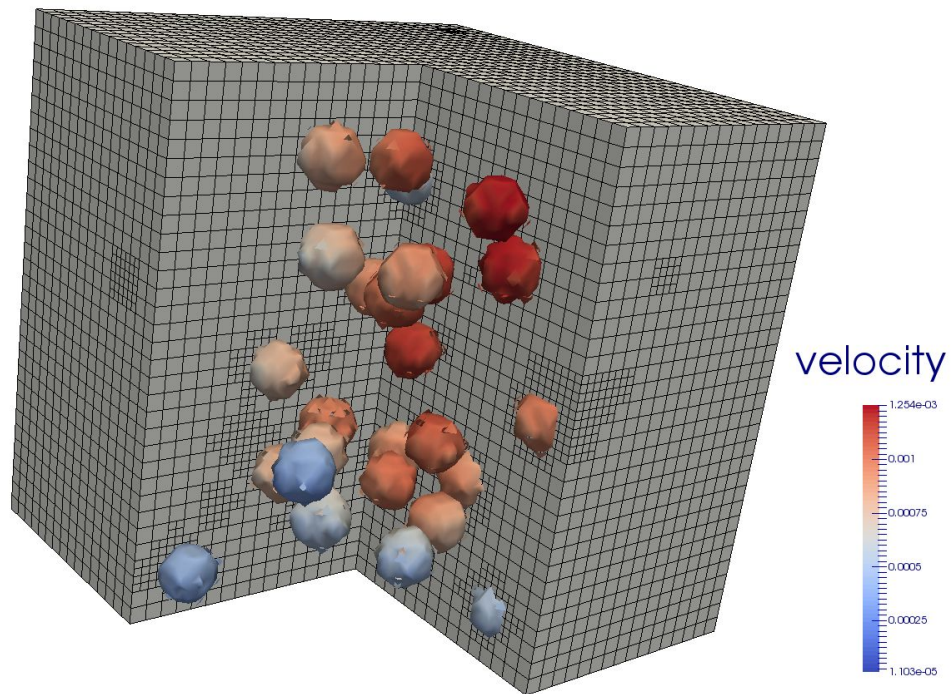
The plugin came first since I needed it for one of the cookbooks. This plugin uses the strain rate field (the norm of the tensor to be precise) as an indicator for mesh refinement. It has been committed and a test has been added. It is particularly useful when one wishes to refine the mesh in the vicinity of shear bands occurring when visco-plastic

rheologies are used.



The cookbook which makes use of this plugin is a crustal deformation one. It implements a single visco-plastic material (representing the upper crust) undergoing extension or compression for 500kyr. It is shown on the above picture.

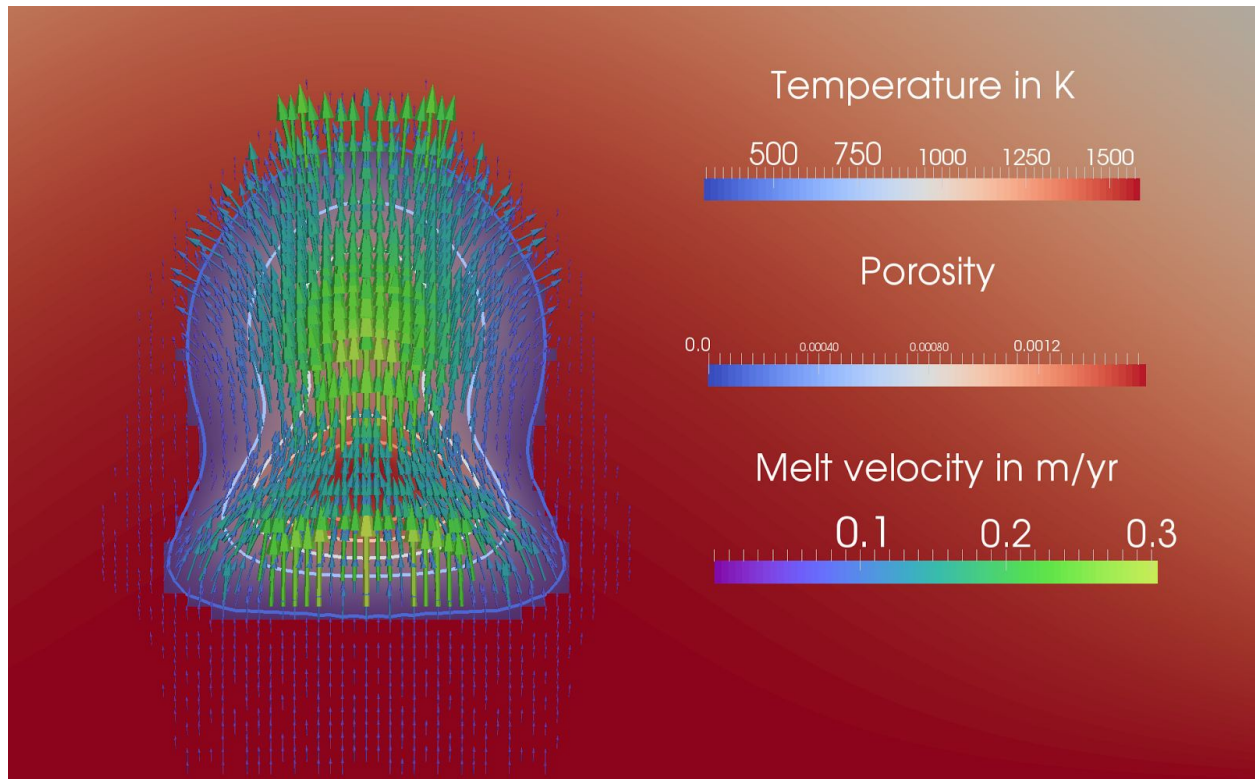
The second cookbook is a not of geodynamical (why not? sinking xenoliths or rising in a magma!!!) nature. It is an extension of the Stokes sphere problem. However, we now have to deal with 75 sinkers randomly distributed in the unit cube. The higher the viscosity contrast with the background fluid, the harder it is to solve the system. A cookbook is being written, but needs input from Wolfgang for high resolution runs.



## Juliane Dannberg

Changed: The heating models have a new structure now: Instead of the implementation of all of the heating terms in the assembly, there is a heating plugin for each model now that can be used both in the assembly and the postprocessors, and a new heating model manager that combines the plugins by adding the individual heating terms. This makes the heating models more flexible and makes it easier to change the exact formulation or use any simplifications such as only using a constant density or only the static pressure. These changes also made it possible to calculate the shear heating more accurately.

In addition, I worked on melt migration in Aspect and we are now able to run models with melt migration and melt generation in dependence on temperature and pressure. This means that the melt does not only influence the material parameters, such as the viscosity, but also moves with a different velocity than the solid, determined by the Darcy flow law.



## Robert Myhill

ASPECT now contains several constants relative to rheology and the Earth, which will serve as a useful reference library and standardise the many approximations made by the ASPECT community. These include the gas constant and internal geometries and conditions (radius, mass, gravity) inside the Earth and Mars.

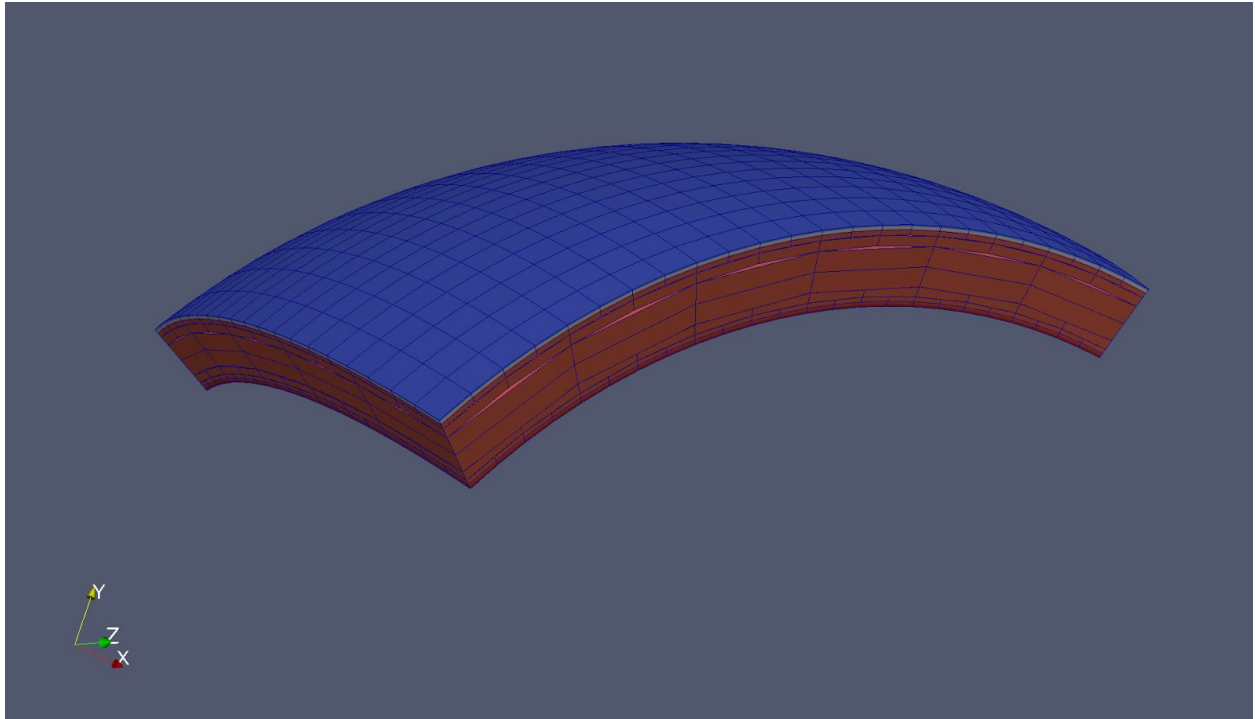
Earth's deformation occurs via multiple creep mechanisms, the most common of which are diffusion and dislocation creep. ASPECT now contains a new material model which contains a generic implementation of diffusion and dislocation creep. This implementation enables the user to input a number of compositional fields with different properties, and a variety of schemes by which to average the resulting viscosities.

ASPECT recently underwent an overhaul of the material model system, which significantly simplified the creation of new material models. The old multicomponent and simple compressible models have now been updated to reflect the new structure, and should therefore become useful templates for new models.

In many studies, we are interested in dynamics within quite a small region of the Earth, but one where spherical geometry remains important. Such situations include regional tectonics and subduction models, or those which use plate motion data. In such situations, using a box or

shell is often either inappropriate or an excessive use of computational resources. ASPECT now contains a new geometry model called “chunk”, which takes latitude, longitude and radius bounds as input. Spherical shell boundary and initial conditions are now also implemented for this geometry.

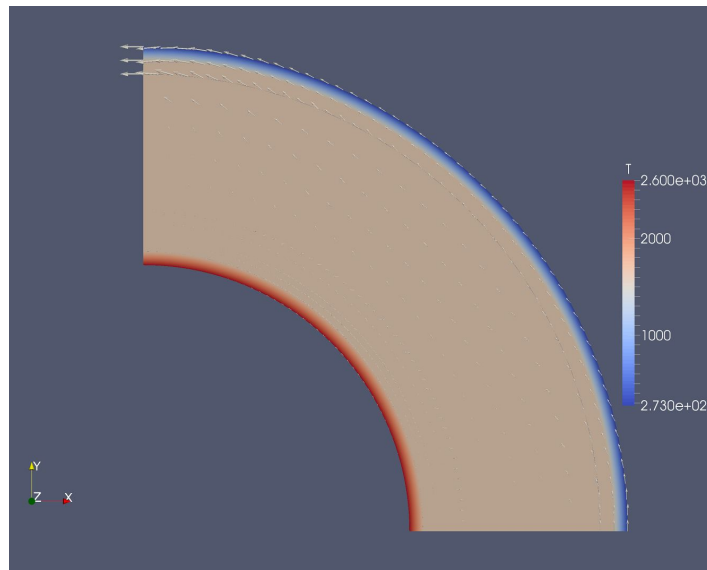
(This model is based on much groundwork by D. S. Stamps, W. Bangerth and M. Fraters.)



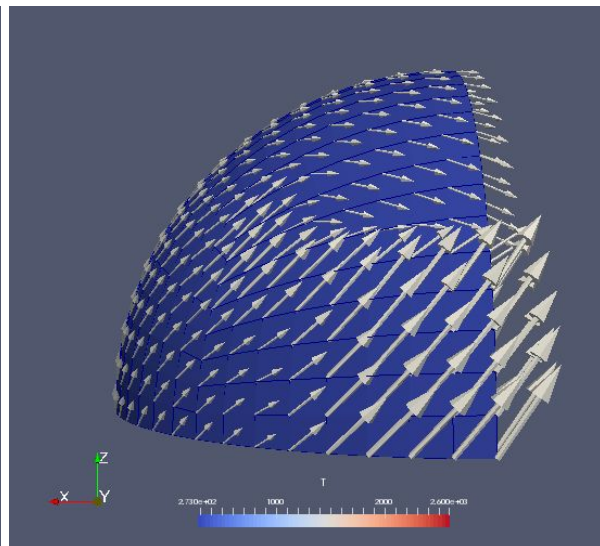
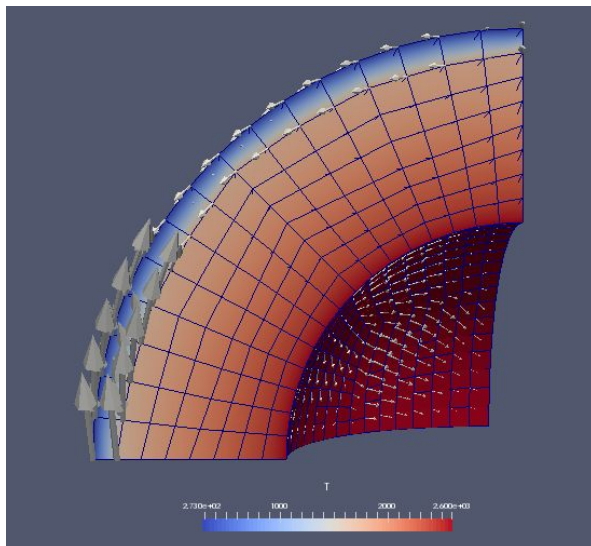
An example of the new “chunk” geometry for the Earth’s upper mantle, with bounds  $[90^\circ\text{E}, 150^\circ\text{E}]$  and  $[10^\circ\text{S}, 30^\circ\text{N}]$ .

## Eva Bredow and Rene Gassmoeller

We worked on the GPlates plugin during the week and restructured it in the form of the AsciiData plugin. Then we started to change it in a way that it can be used for local box geometry models as well as for spheres. Now it is possible to use it for parts of a sphere (e.g. a quarter of a 2d spherical shell) and to apply the GPlates velocities at the side boundaries of the model. Along the depth of the lithosphere on the left and right boundary, the velocity of the appropriate location on the surface is applied and below the lithosphere it is set to zero (see first picture).

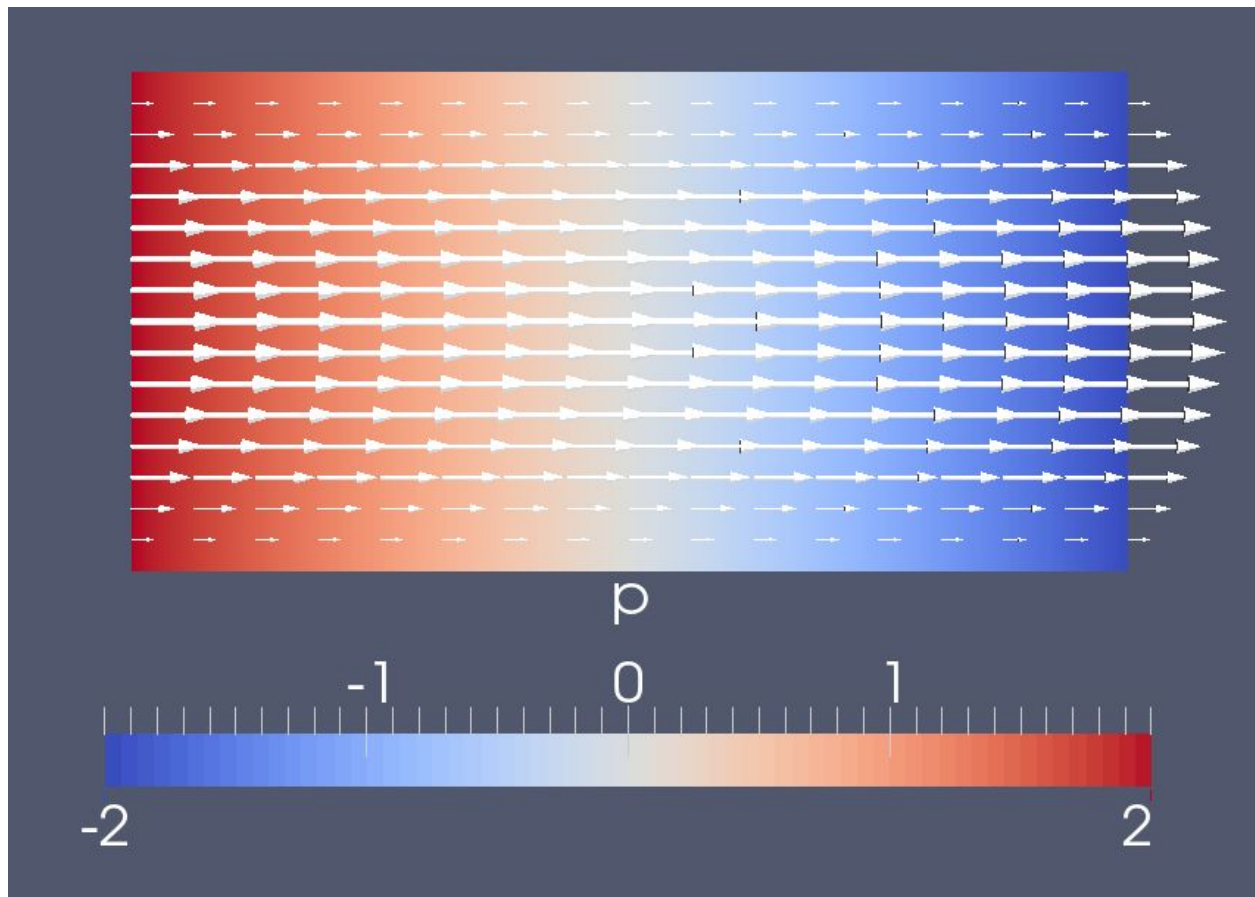


The Gplates plugin also works on 3D spherical geometries, but the rotation to a specific location on the Earth does not work yet. Unfortunately, it does not work for box geometries (the mapping procedure is not implemented correctly yet), and therefore it is not ready to be merged. Considering the new curved geometry models the mapping might not longer be necessary, but this will be evaluated after the hackathon.

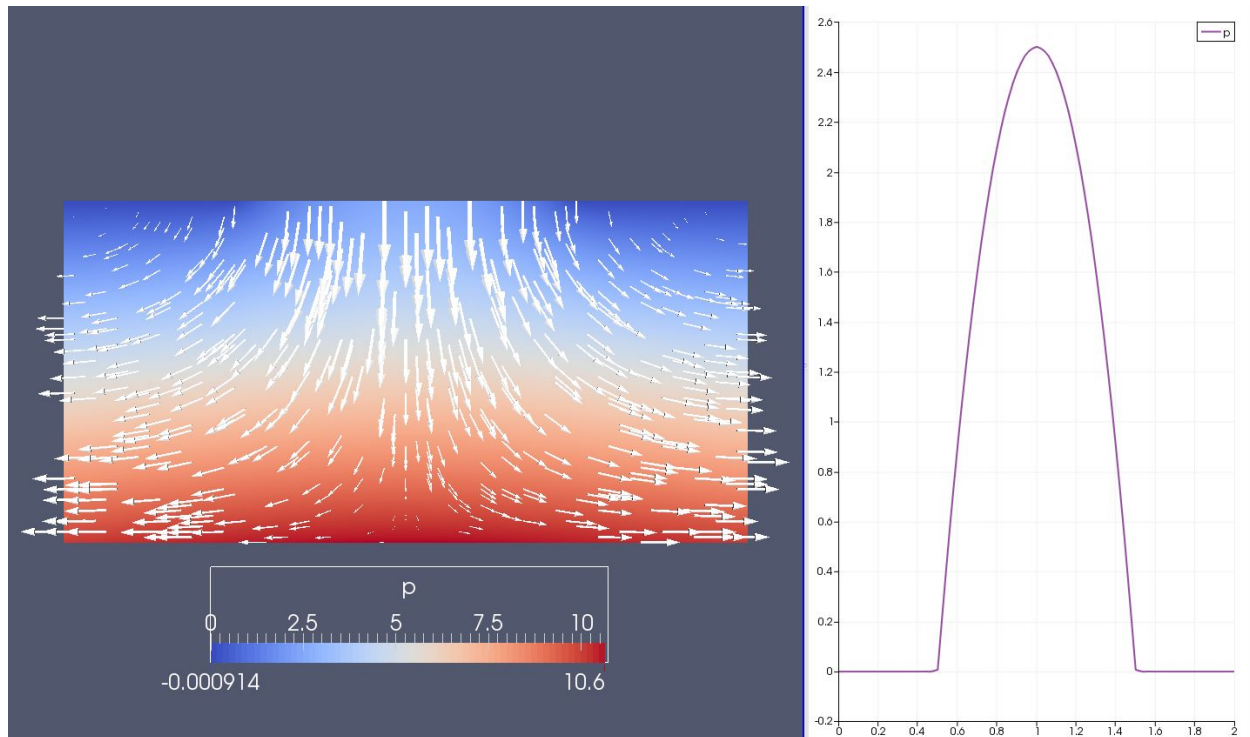


## Anne Glerum

Wolfgang's prescribed traction boundaries now have xyz selectors. Below is an example of Poiseuille flow, where we prescribe the normal component of the traction and set the tangential velocity component to zero on the vertical boundaries. As expected, the resolved velocity field is the same as when prescribing the velocity on the boundaries.



With Carolyn I've started thinking about a possible ice sheet loading cookbook using the prescribed traction boundary conditions. Below a first model where we prescribe a parabolic surface pressure to mimic the loading by an ice sheet (see right plot) and prescribe the lithostatic pressure to the vertical boundaries. The produced velocity vectors and pressure field are shown on the left.



In the iterated\_IMPES solver, we're now rebuilding the preconditioners for every nonlinear iteration. For the tests/iterated\_IMPES\* models, this results in less linear temperature iterations and a smaller "Total relative nonlinear residual". The iterated\_Stokes solver now uses the same initial residual as iterated\_IMPES, so that convergence can be monitored better.

There is now a one-material, Drucker Prager frictional plasticity material model that can be used to model crustal deformation, see the cookbook added by Cedric.

A new geometry model provides additional boundary indicators for the lithospheric part of the left and right vertical boundaries (and the front and back boundaries in 3D). This way one can for example prescribe a velocity to the lithospheric plates and use open boundary conditions for the mantle underneath. I would like to change the way the subdivided hyper rectangle grid is setup however, so I marked the pull request WIP.

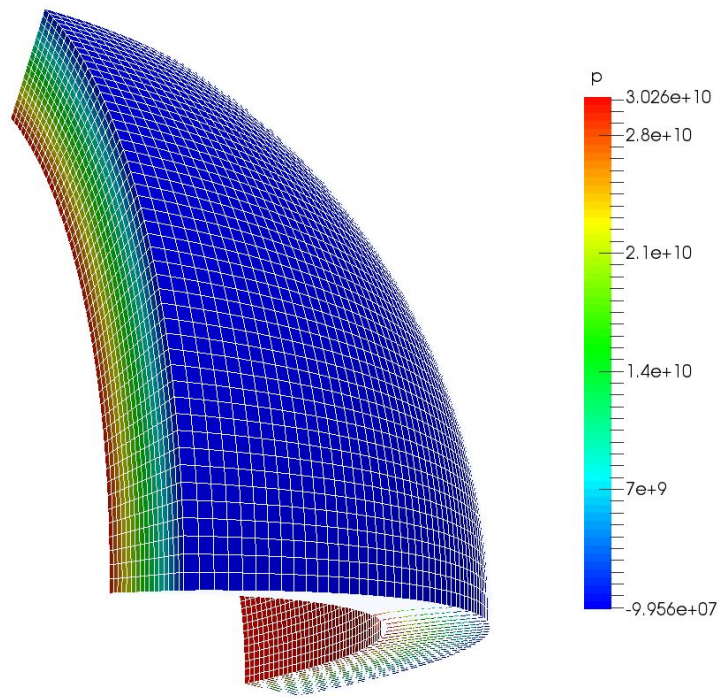
## Menno Fraters

There is now a 'composite' material model which implements all the material averaging schemes which wolfgang implemented, except for the Q1 scheme, and implements three more averaging schemes. A composite material model is a material model which uses the values of another material model and performs an operation on it. The new averaging schemes implemented are three Normalised Weighted Distance (NWD) averaging schemes, NWD arithmetic average, NWD geometric average and NWD harmonic average. Normalised Weighted Distance average means that the average is a weighted average which uses the the

normalised distance to calculate the weights. The advantage of these methods is that values at the quadrature points are not forced to be exactly the same, but are allowed to differ in contrast to the previously implemented arithmetic, geometric and harmonic averages. The weighting of each quadrature point is calculated by a spanning a bell shaped curve around it and defining a limit of the bell shaped curve.

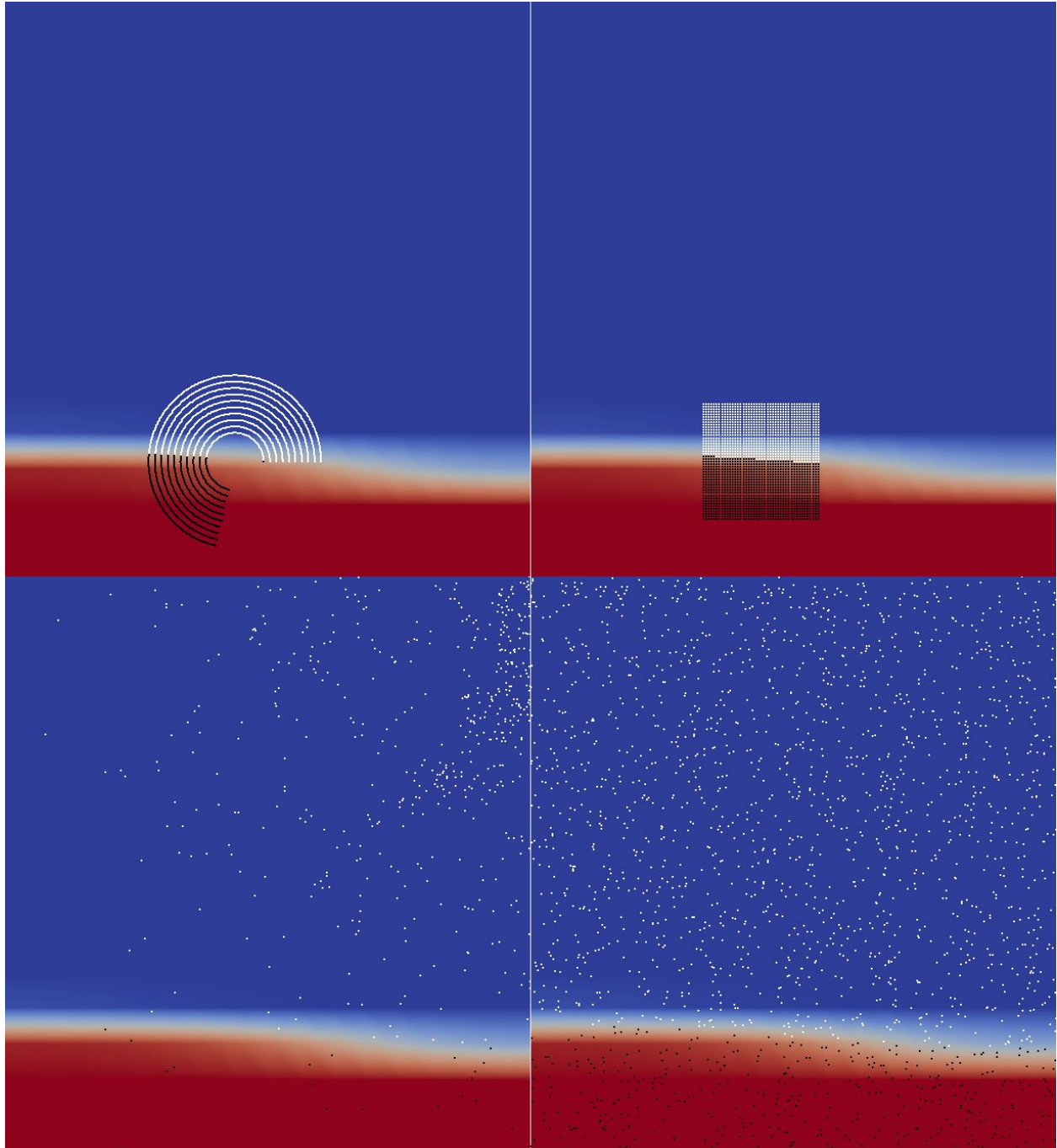
A preliminary version of the ellipsoidal geometry model has been made available (of which the base was made by D Sarah Stamps and Wolfgang Bangerth). Some work has been done on cleaning and expanding it. One of the new feature in the model is that it will be possible to chose areas which are not aligned to the coordinate system.

Some work on a plugin which allows to set the minimum and maximum refinement level based on parameters such as position, temperature, density, composition, viscosity etc.



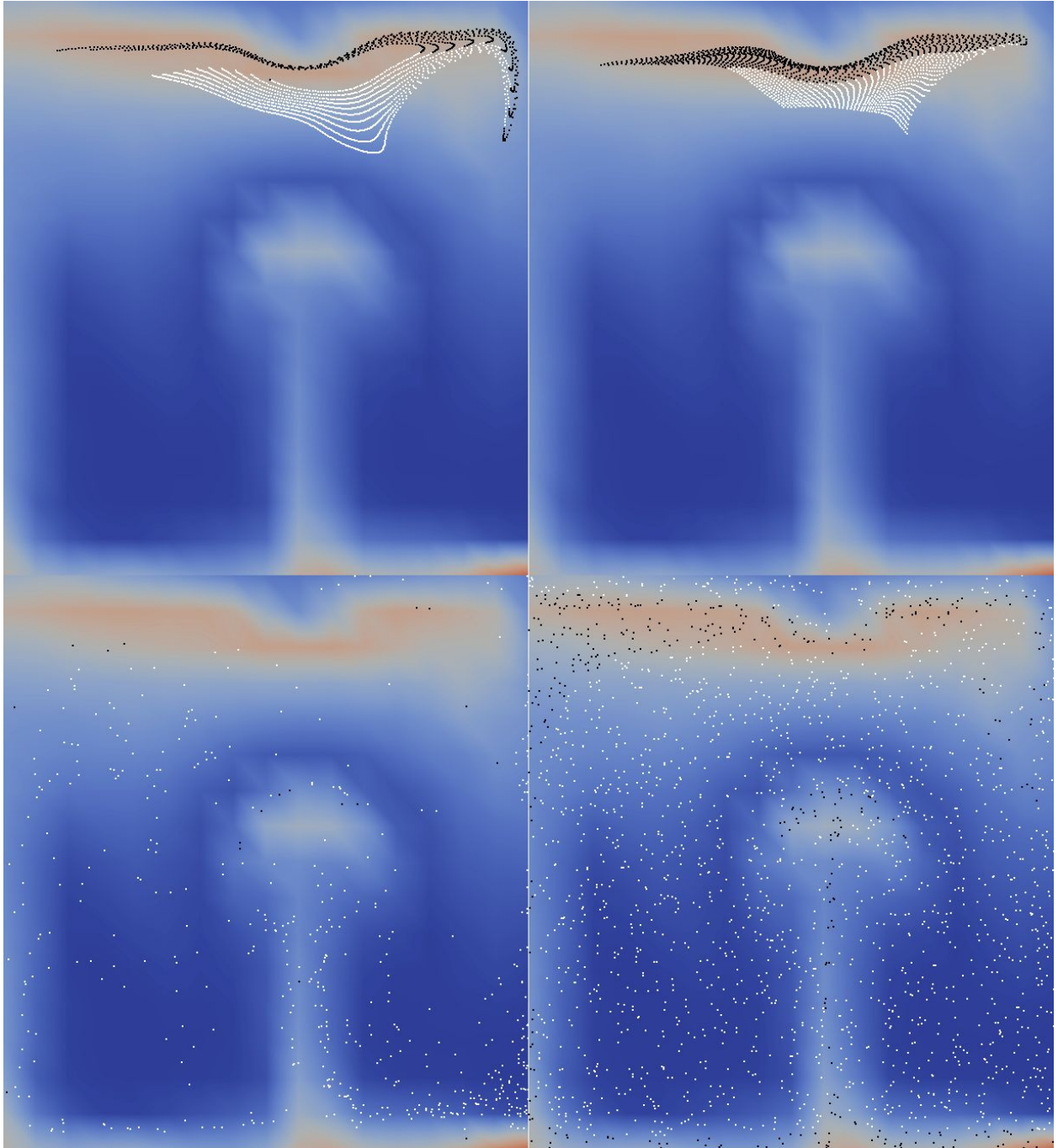
## Rene Gassmoeller and Gerry Puckett

Besides from the technical points mentioned in the list of participants above we made the particle system more flexible and conformant with the usual ASPECT structure. Due to the large amount of code this part is not ready for merge yet, but the new system allows for many applications to use tracers to track the flow. Examples for new particle generators are shown below on a very coarse mesh.



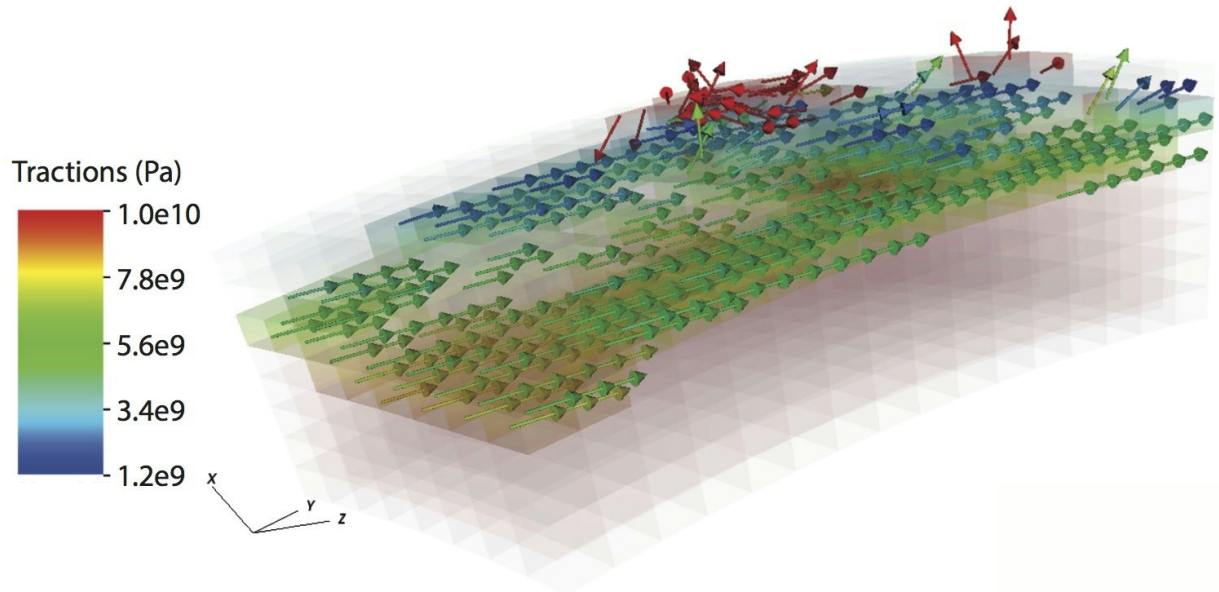
Additionally each particle can now carry user-defined properties, to make them more useful. Examples for such properties are:

- an user-defined spatially variable function that gets assigned to the tracers at the beginning
- the initial position of the tracers to track their movement since the model start
- the initial composition of the tracers to compare to the diffusion of the compositional field
- the current pressure-temperature condition to track the pT-path of a particle



## Wolfgang Bangerth and Sarah Stamps

We wrote a postprocessor that is extended from previously implemented stress postprocessor to output tractions at the user-defined lithosphere-asthenosphere boundary (LAB). The figure below shows the traction vectors at the cells that surround the LAB for a coarse global refinement of 3.



## Sarah Stamps and Jonathan Perry-Houts

Updated the ASPECT installation guide for TACC Stampede cluster. Instructions are now in the aspect.git under doc/install. The guide will also be made available on the CIG wiki.

## Ying He

- 1, Wrote codes using deal.ii to solve Time-dependent Temperature advection diffusion equation using Local discontinuous galerkin method.
- 2, Wrote codes by replacing the temperature equation in step-31 by using the DG temperature solver mentioned above for the advection only problem.
- 3, Added a postprocess limiter after each time step to the temperature solution to ensure the temperature satisfying some prescribed global maximum/minimum value
- 4, Ongoing: adding WENO limiter to reduce the oscillation when using higher method

Numerical example and results:

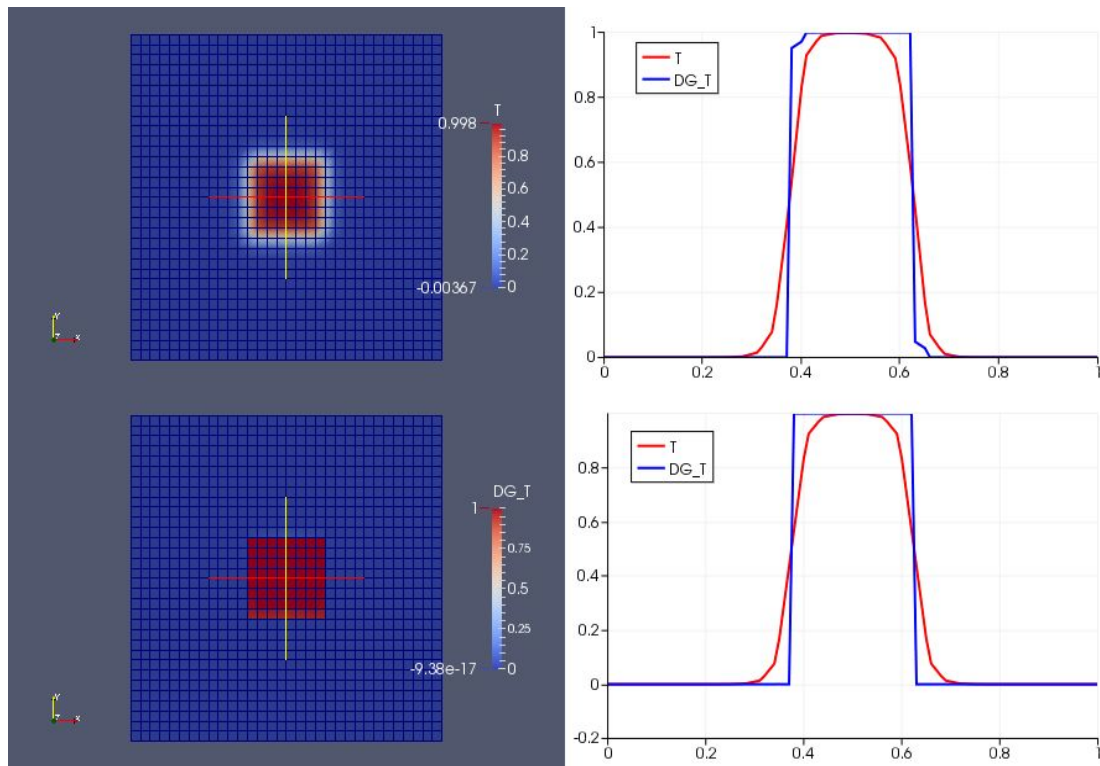
- 1, a detail description of the test problem

[https://www.math.ucdavis.edu/~yinghe/Hackathon2015\\_report.pdf](https://www.math.ucdavis.edu/~yinghe/Hackathon2015_report.pdf)

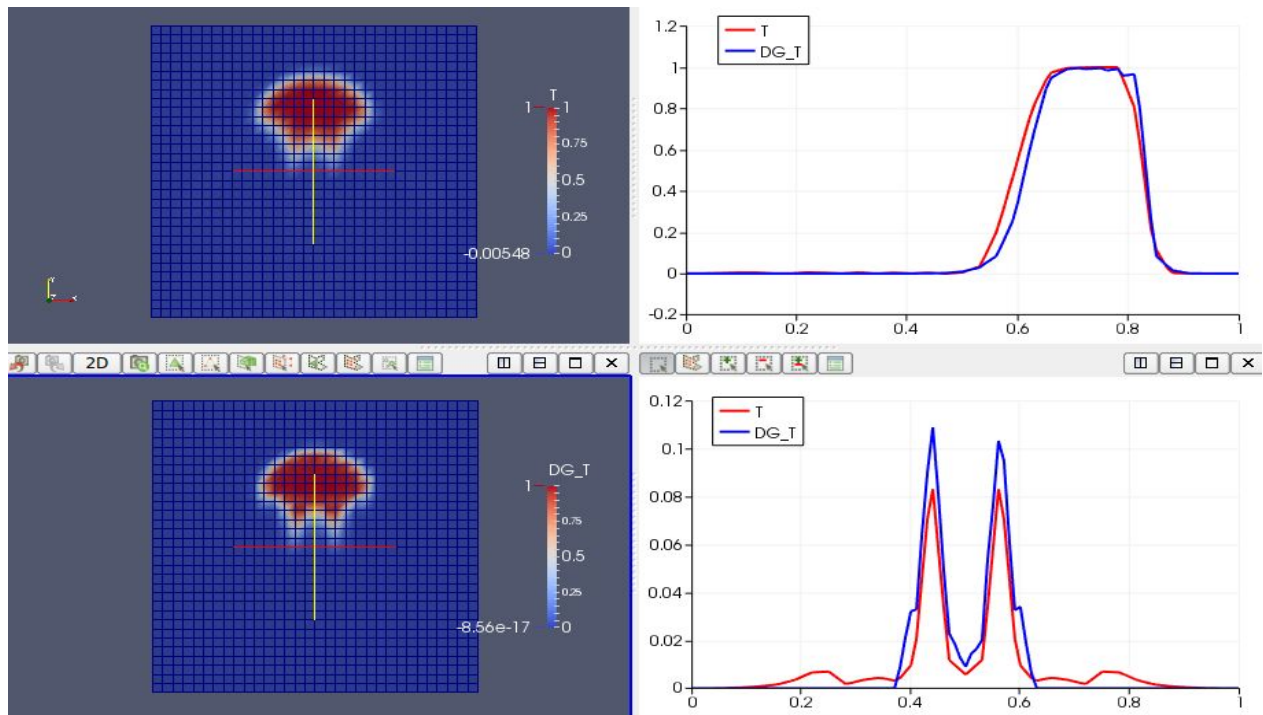
- 2, an animation of the numerical result in time

[https://www.math.ucdavis.edu/~yinghe/DGQ\\_FEM\\_Advec\\_T\\_30.gif](https://www.math.ucdavis.edu/~yinghe/DGQ_FEM_Advec_T_30.gif)

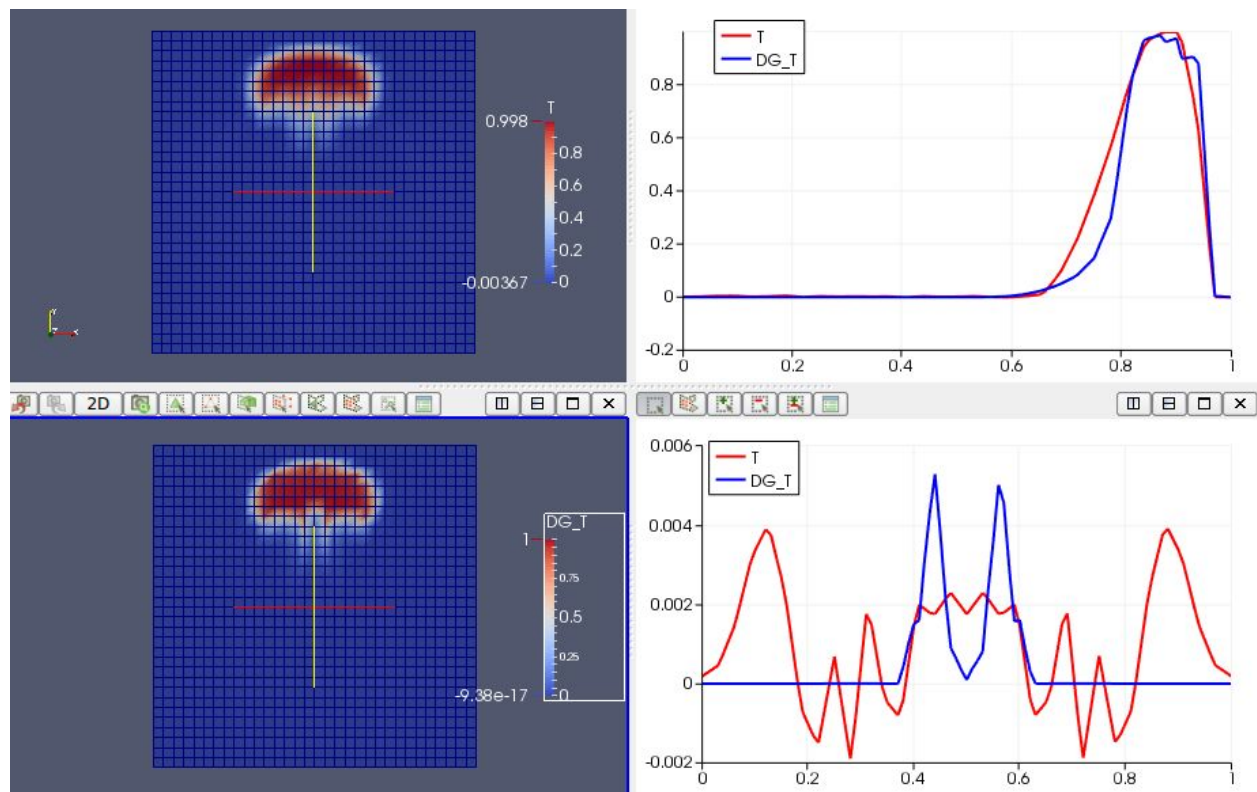
Figures:  
Time  $T=0.001$



Time  $T=5$



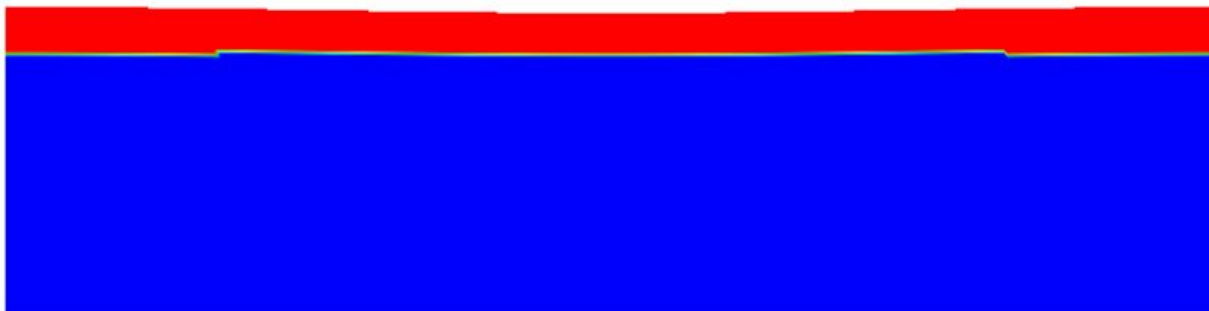
Time  $T=10$



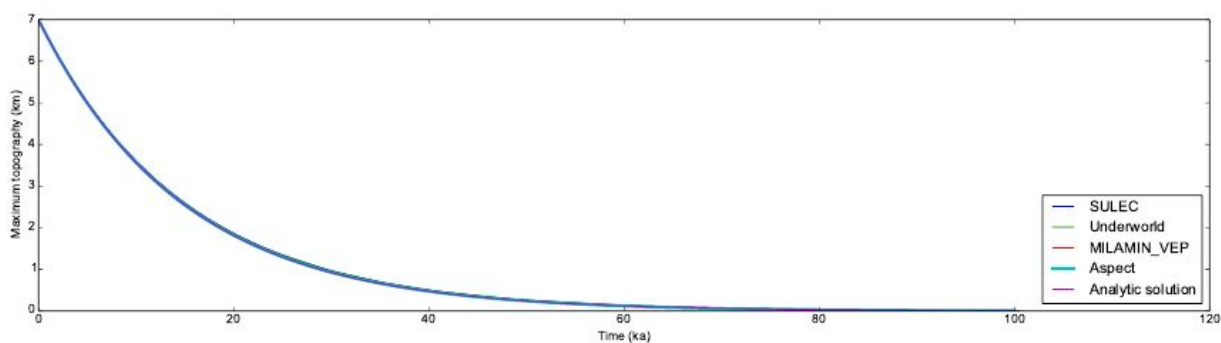
## Ian Rose

I worked on adding free surface benchmarks from Cramer et al. (2012), as well as an accompanying benchmark write-up in the manual. Free surface computations are quite sensitive to choices of resolution, time stepping, and remeshing algorithms. Additionally, without some form of stabilization at the free surface they are likely to exhibit a serious sloshing instability, sometimes known as the “drunken sailor instability.” ASPECT currently implements a stabilization scheme proposed by Kaus, Mulhaus, and May (2010), though we are examining other schemes.

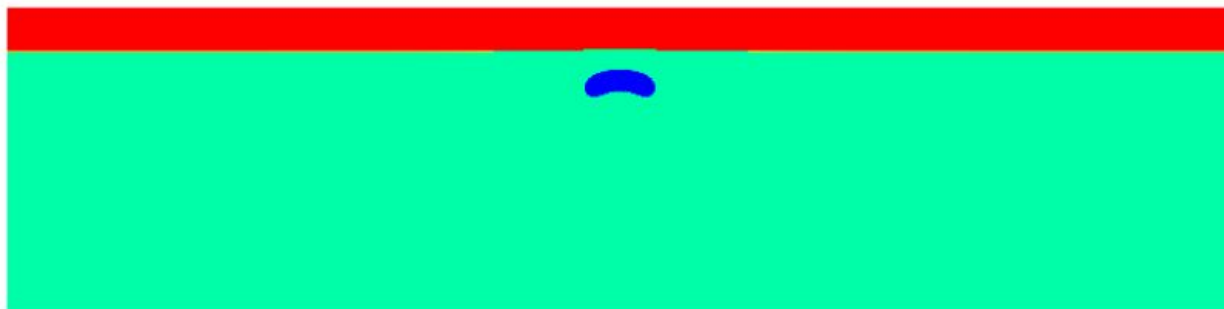
The first benchmark involves relaxation of initial sinusoidal topography. There is a semi-analytical solution to this problem, which makes it a good starting benchmark. A higher viscosity lid with initial topography sits on top of a lower viscosity mantle, as shown below.



Over  $\sim 100$  ka the topography relaxes. The results of Aspect are essentially indistinguishable from those of other free surface codes participating in the benchmark:

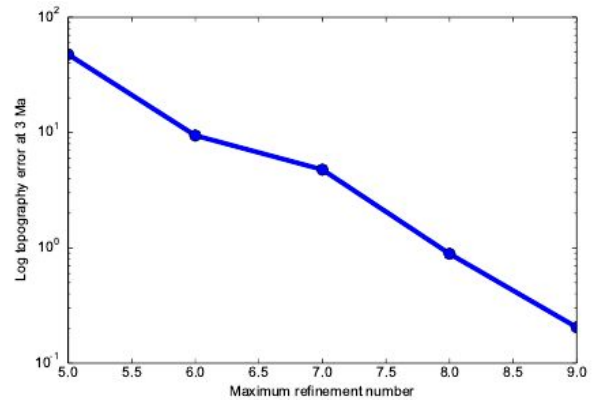
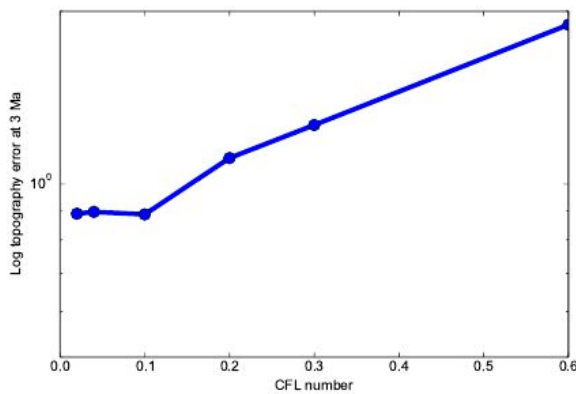
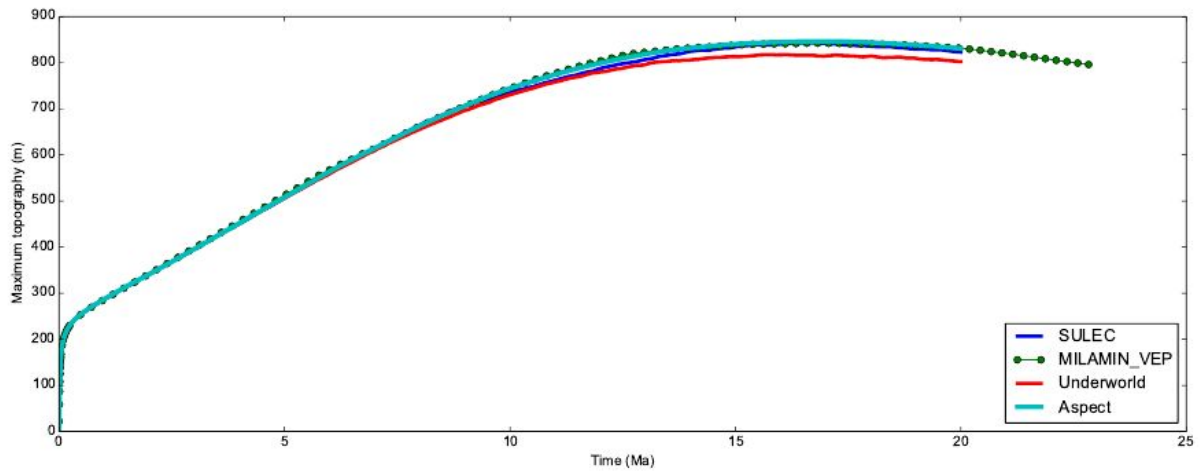


The second benchmark is much more challenging. Again, there is a high viscosity lid on a lower viscosity mantle, but this time there is a blob of buoyant material which rises, deflecting the topography upwards.



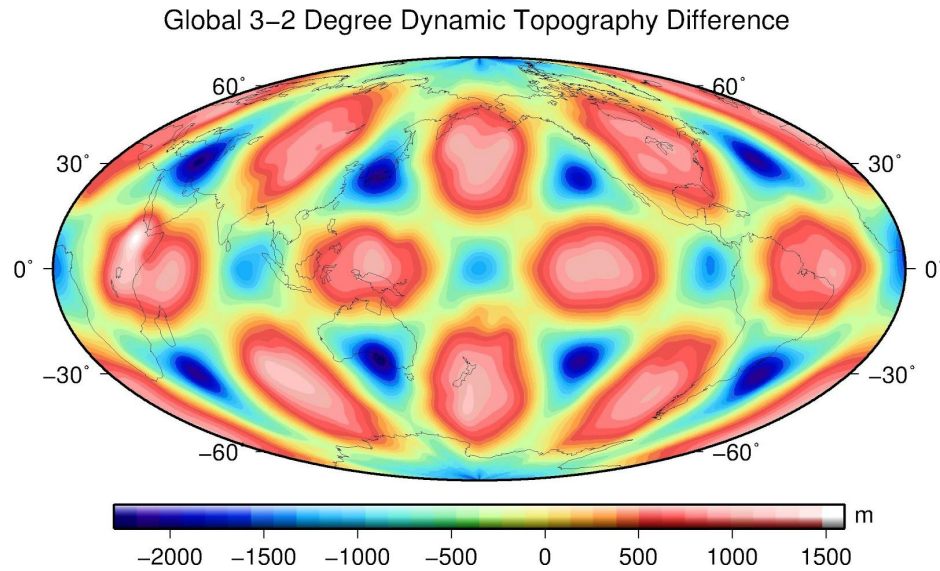
Relatively low resolutions qualitatively reproduce the benchmark, but it is not until quite high resolution and small time steps that the results converge to a stable value. Shown below are a

comparison with other participating codes, as well as a convergence table with timestep and mesh resolution.

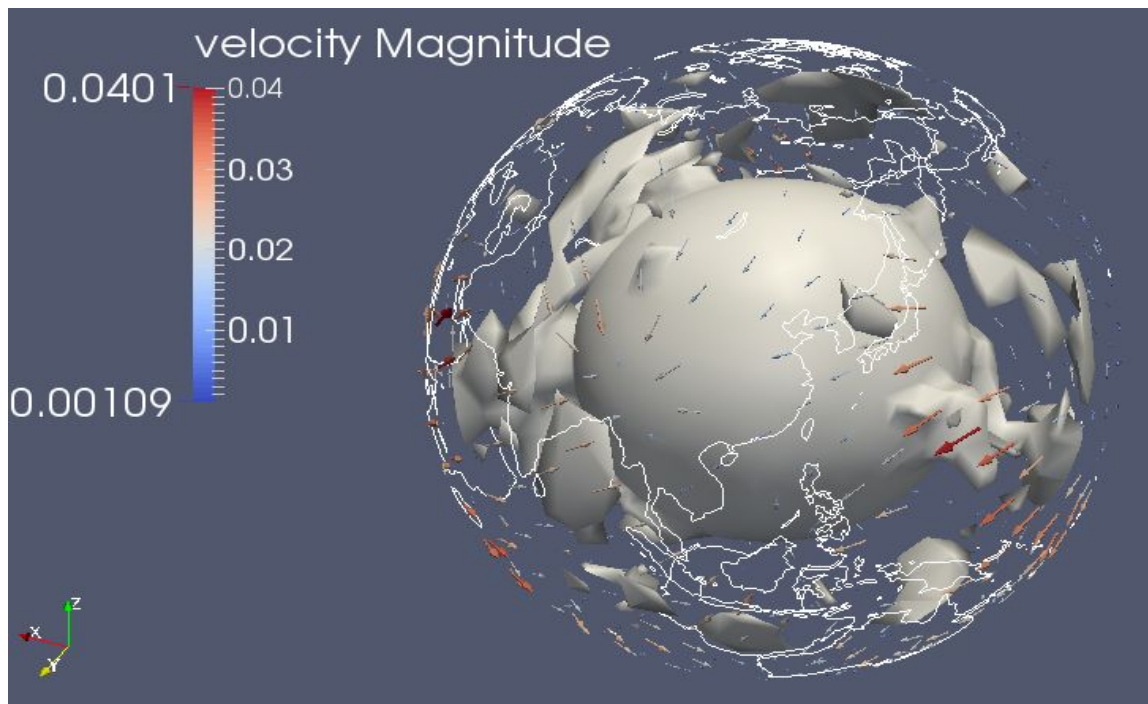


## Shangxin Liu

Part of my work is to compare the dynamic topography resulted from different finite element orders. When I made the topography difference between different orders, I found an interesting mesh issue of aspect as shown in the following figure:

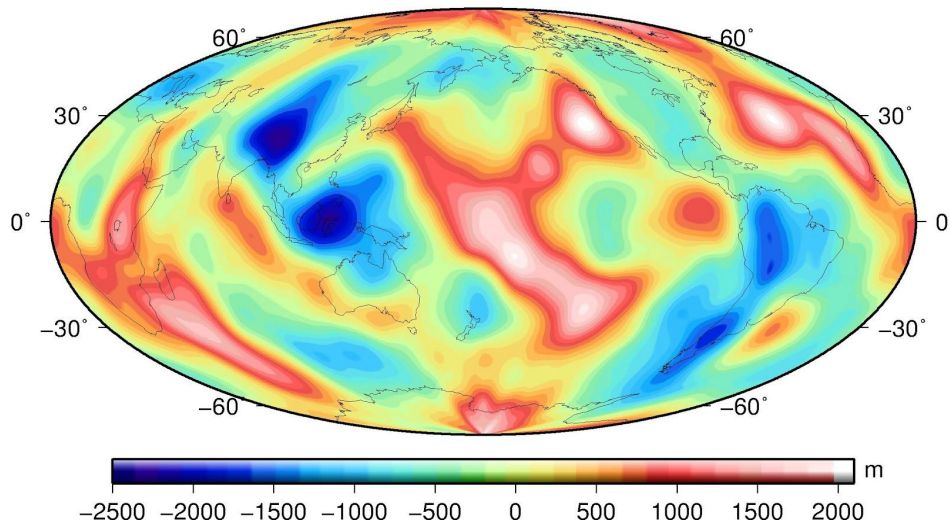


I also put SAVANI, a global radial anisotropy tomography model, into ASPECT as a new temperature perturbation initial condition. Here is an example of the Earth subsurface flow field driven by SAVANI perturbation with an interior isotherm 1700 K, displaying some upwelling hot material in the mantle.

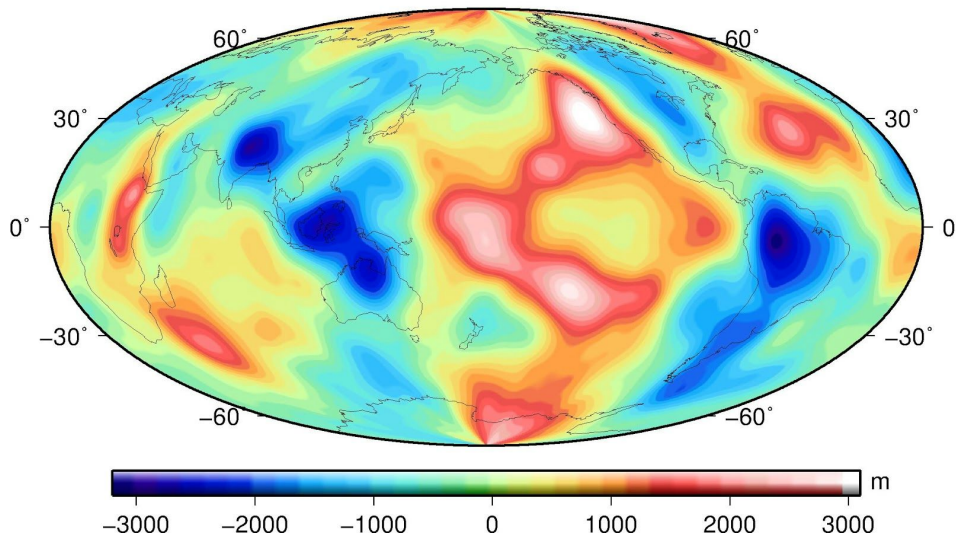


The following two figures are the global dynamic topography computed from SAVANI and S40RTS. The two patterns are in general similar but different in some local regions. For example, they all reflect positive anomaly at Eastern Africa Rift and Mid-ocean ridges. However, they differ from each other to a certain extent on Indian-Australian plate and South American plate.

Global Dynamic Topography from SAVANI Perturbation



Global Dynamic Topography from S40RTS Perturbation



In addition to code stuff, I summarized a step-by-step ASPECT installation workflow on Linux machine and shared it on the mailing list. It may be helpful for the future users to deal with ASPECT installation difficulty:

<http://lists.geodynamics.org/pipermail/aspect-devel/attachments/20150523/66b9a290/attachment-0001.pdf>