ASPECT Hackathon 2016

Final report

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Introduction

The 2016 ASPECT hackathon was held June 24th to July 2nd 2016 in Davis, CA and Lake Tahoe, CA, with 23 participants from the United States, Canada, the United Kingdom, the Netherlands, and Germany.

The following pages contain a list of participants and their interests and goals for this workshop, followed by a list of projects they worked on with short descriptions of what progress they made. The last section contains a set of statistics that collect (impressive!) information about the growth of ASPECT over the course of the hackathon.

Participants and areas of interest

Name, affiliation, email	Goals and interests for this hackathon
Wolfgang Bangerth Texas A&M University (future: Colorado State University) bangerth@math.tamu.edu	1. Help others 2. Review most code submissions 3. Fix bugs others may find 4. Get people involved
Timo Heister Clemson University heister@clemson.edu	1. Help others, code review 2. Equation / Approximations 3. Citations for ASPECT 4. Stokes Solver improvements
Lorraine Hwang UCD ljhwang@ucdavis.edu	1. Den mother 2. Write papers 3. abstract WSSSPE4 4. SAGA->ASPECT: https://github.com/geodynamics/aspect/issues/914
Rene Gassmöller Texas A&M University gassmoeller@math.tamu.edu	1. Help others, code review 2. Equation / Approximations / Assemblers 3. Particle improvements 4. Help with Geoid
Gerry Puckett UCD egpuckett@ucdavis.edu	1. Testing of Binary I/O PR #872 2. Finish PR #861 (particle injection functionality) 3. 2D Convection Rolls cookbook using the Turcotte stability analysis example
Harsha Lokavarapu UCD	4. 2D multicomponent model that is able to have two density equations in each component

lokavarapuh@gmail.com	5. Create O(N) particle generation algorithm for uniform box 6. Create Richardson extrapolation convergence test 7. Test convergence of active particle algorithm with falling box or falling circle?
Juliane Dannberg Texas A&M University dannberg@math.tamu.edu	1. Help others, code review 2. Melt transport improvements 3. Equation / Approximations / Assemblers 4. Nonlinear solvers? 5. Traction boundary conditions...
Ian Rose UC Berkeley ian.rose@berkeley.edu	1. Use total Lagrangian formulation for free surface 2. Geoid 3. Think about surface processes in spare time
Louise Kellogg UC Davis kellogg@ucdavis.edu	1. Thermo-chemical convection 2. Spherical test cases 3. SAGA -> ASPECT 4. Learn stuff 5. Grand Poobah of the Benevolent Society of Aspect User-Developers.

Benjamin Smith
Clemson University
bjs2@g.clemson.edu
	1. Help others (as much as I can)
	   a. ASPECT / GitHub
	2. Citations for ASPECT
	   a. SAGA??

Jacky Austermann Harvard University jaustermann@fas.harvard.edu	1. Geoid 2. Heatflux as visual postprocessor 3. Speed up initialization of tomography models 4. Backward advection 5. Maybe … read in tomography from grid (as outputted on IRIS website) 6. Maybe … plate-like boundary condition (enforce rigid-body rotation of plates)
Shangxin Liu Virginia Tech shangxin@vt.edu	1. Improve Geoid code to work with AMR 2. Global slab model 3. Complex lithosphere structure (incorporating weak plate boundaries, differences between ocean/continent, oceanic plate age) 4. Fix some bugs
Ying He UC Davis	1. 3D implementation of DG bound preserving limiter

yinghe@math.ucdavis.edu	2. Write a section about the DG bound preserving limiter for the ASPECT manual 3. Other local limiter for DG advection equation
Anne Glerum Utrecht University a.c.glerum@uu.nl	1. Add traction boundary conditions plugins 2. Topography from file for ellipsoidal chunk 3. Velocity singularities for chunk 4. Read in tomography from file?
Menno Fraters Utrecht University m.r.t.fraters@uu.nl	1. Get Newton nonlinear solver working 2. Topography for ellipsoidal chunk 3. Add spacedim to aspect 4. Move ellipsoidal equations to utilities
Sam Cox University of Leicester spc29@le.ac.uk	1. Cookbook illustrating dG method 2. Explore effect of dG on Stokes solve and assembly times 3. Understand current Stokes preconditioner and solver process
Jonathan Robey UC Davis jmrobey@ucdavis.edu	1. Clean up, debug Volume of Fluid interface tracker 2. Work on small issues
Anthony Osei Tutu GFZ Potsdam oseitutu@gfz-potsdam.de	1. Improve and benchmark Geoid postprocessor
Tahiry A. Rajaonarison Virginia Tech trajaona@vt.eu	1. Initial temperature condition derived from both global and regional tomography

Report on areas worked on

Coupled magma/mantle dynamics

(Juliane Dannberg, Timo Heister)

We have finalized our implementation of coupled magma/mantle dynamics, and merged it into the developer version of ASPECT. ASPECT now allows solving additional equations describing the behavior of silicate melt percolating through and interacting with a viscously deforming host rock. This includes the effect of melt on material parameters, such as viscosity, permeability

etc., compaction and dilation of the matrix when melt flows through, heat transport by melt, melting, freezing, and compositional changes due to melt migration.

This addition allows to model a number of phenomena related to coupled magma/mantle dynamics such as shear bands, solitary waves, melt migration in mantle plumes, and global-scale models with melt transport (see below). The implementation in ASPECT also includes a number of benchmark cases and cookbooks.
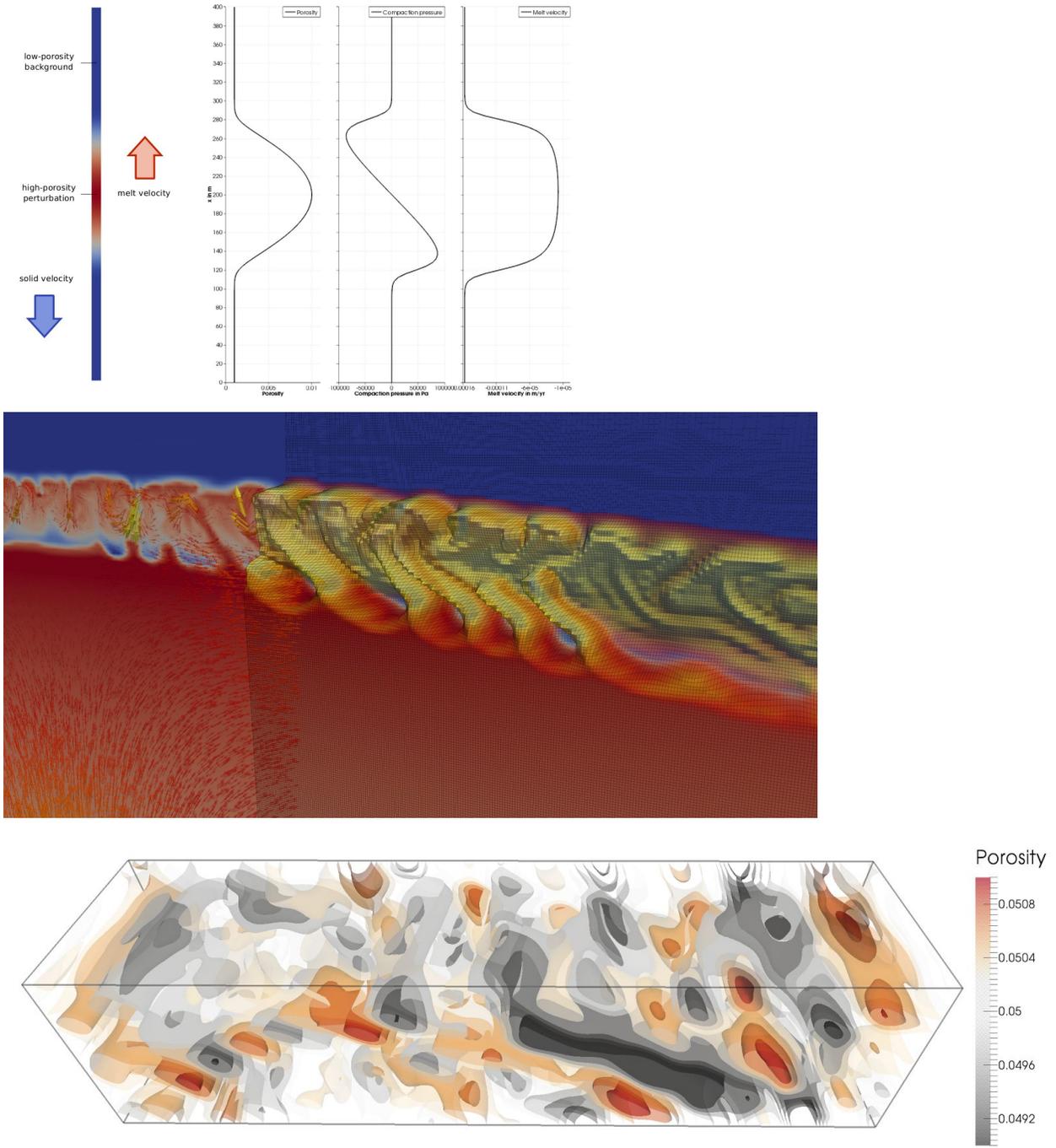
Example of models with melt migration is ASPECT: solitary waves, melting in a mantle plume, shear bands.

Approximations of the governing equations

(Timo Heister, Juliane Dannberg, Rene Gassmoeller)

There are a number of common variations to the Stokes and energy conservation equations that are frequently used for mantle convection. For example, one frequently finds references to the anelastic liquid approximation (ALA), truncated anelastic liquid approximation (TALA), and the Boussinesq approximation (BA). These can all be derived from the basic equations used in ASPECT via various approximations. The three approximations mentioned all define a reference state for temperature and pressure, and a depth-dependent reference density.
We have implemented these approximations by allowing modifications to the equations that are solved in the code in dependence of which approximation is chosen by the user in the input file:
In places where the approximation uses the reference density instead of the real density, the density parametrization in the material model is called with the reference temperature and/or reference pressure (instead of the real density or pressure), and thus returns a reference density.
This new implementation allows us to run a number of benchmark cases that use these approximations more easily than before, for example the Blankenbach benchmark (see below).
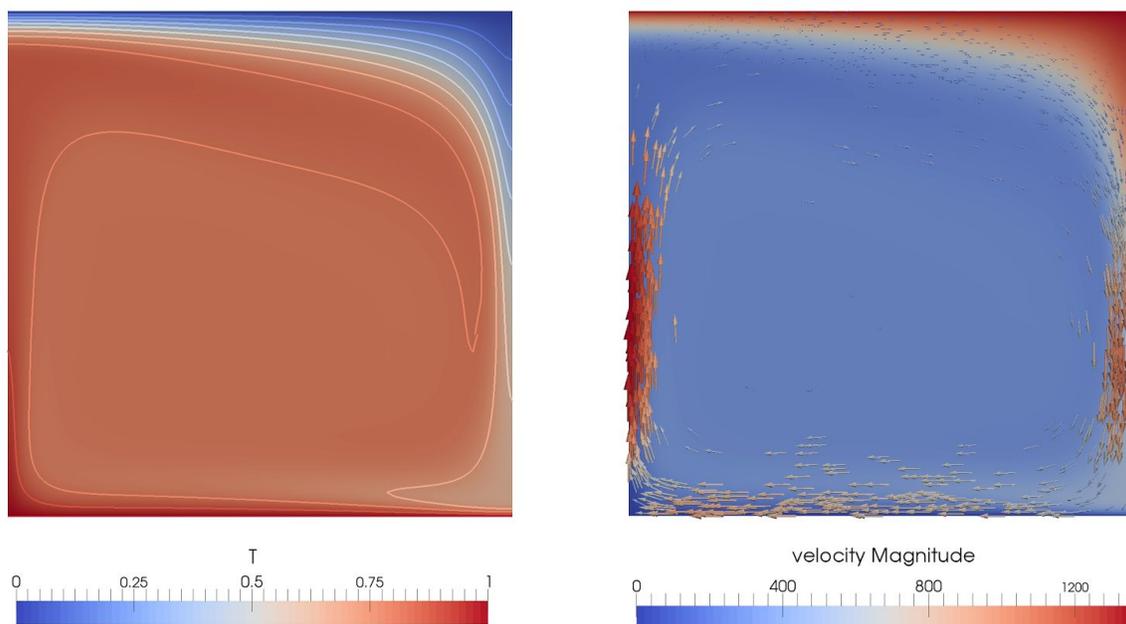

Blankenbach benchmark with temperature-dependent viscosity (case 2a). The left panel shows the temperature, the right panel shows the viscosity, overlain by velocity arrows.

Heat flux map postprocessor

(Jacky Austermann)

The heat flux map postprocessor computes the conductive heat flux density across each boundary. The heat flux density is computed in outward direction, i.e., from the domain to the outside. A postprocessor for the integrated heat flux for each boundary was already part of the previous ASPECT version as part of the heat flux statistics postprocessor. It is now possible to output the heat flux density as a text file for further postprocessing or as part of the paraview / visit visualization. I included this postprocessor (and a figure of the result) in the cookbook "3D convection with an Earth-like initial condition", which uses the S20RTS tomography model to initialize 'Earth-like' convection. The figure below shows the heat flux density for this cookbook at the surface and the core-mantle boundary. Despite the simplicity of this cookbook (e.g. isoviscous, linear rheology, simplified boundary layers etc) it does roughly reproduce the pattern and magnitude of the Earth's heat flux. At the surface a clear correlation with mid-ocean ridges (high heatflow) and continental cratons (low heatflow) is visible. At the core-mantle boundary, least influx comes through the large low shear wave velocity provinces, since they are prescribed (through S20RTS) as already being hot.

Heat flux density (mW/m^2) at the surface

Heat flux density (mW/m^2) at the core mantle boundary
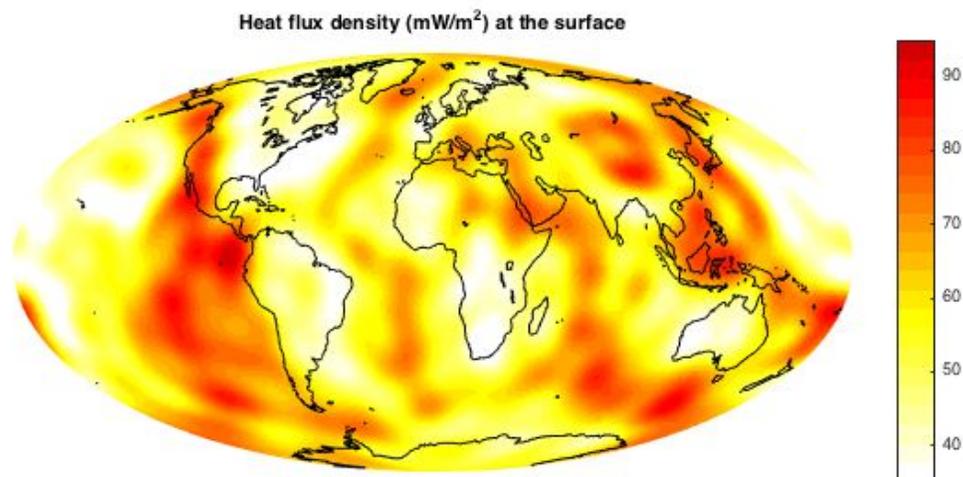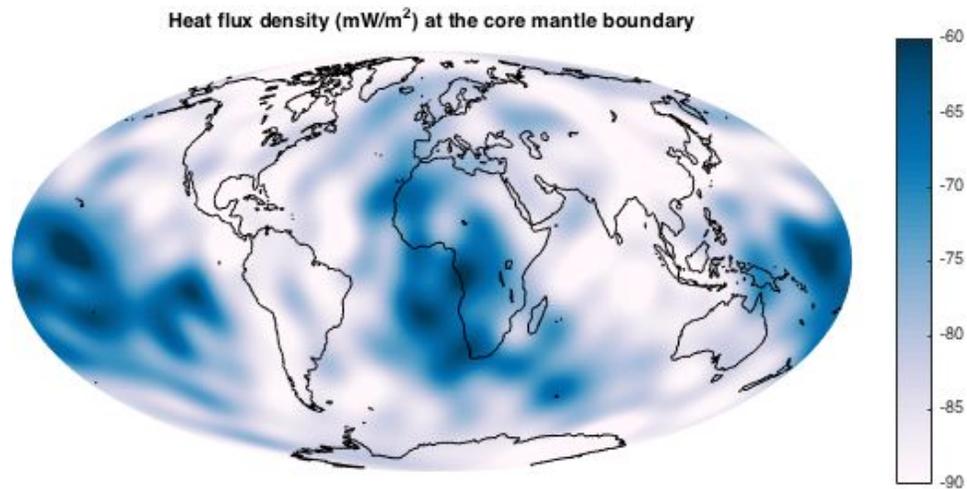
Backward advection

(Jacky Austermann)

I adjusted Aspect to be able to compute backward advection. This can now be done by prescribing negative gravity, which will invert mantle flow. For backward advection it is also advisable to set thermal diffusivity to zero since thermal diffusion is irreversible. An input file that demonstrates backward advection is included in the ASPECT tests folder.

Improving the current dG implementation

(Sam Cox)

I implemented two postprocessors to display memory usage and matrix entry numbers, which will be helpful for debugging and validation. I also made several updates to fix functionality, for example dG with non-planar faces.
A lot of time was spent beginning work on improving the current dG implementation - it is currently very inefficient, allocating far too much matrix space, and there is room to vastly improve this and, consequently, the memory usage. The new postprocessors should help in extending our understanding.
Finally, a cookbook illustrating the dG implementation is nearly ready for review. Below is a comparison of the continuous FEM and dG-FEM solutions for the second composition field in the composition-passive cookbook.
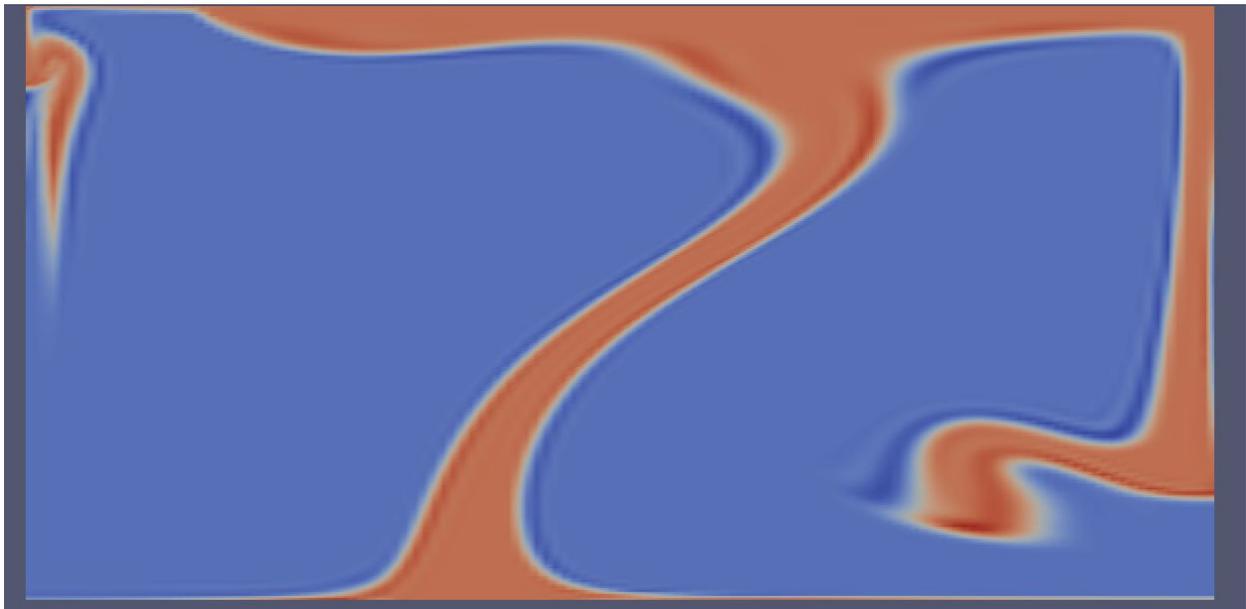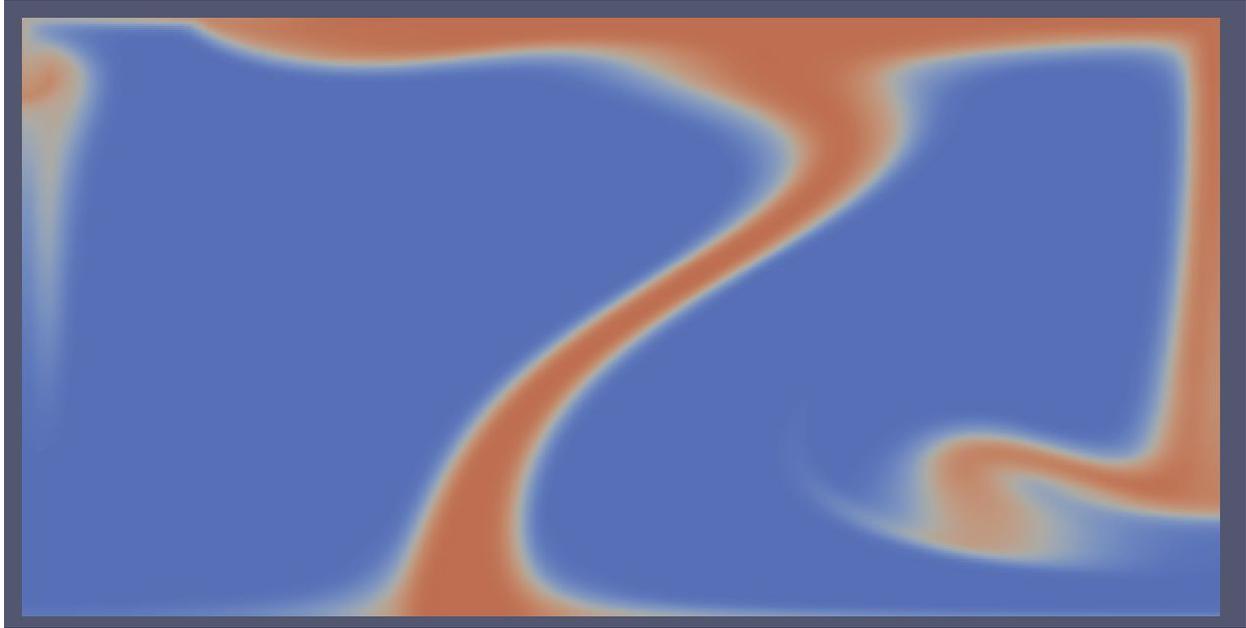
Convection in the inner core

(Juliane Dannberg)

I finished a cookbook about convection in the inner core:
The mechanical boundary conditions for the inner core are tangential stress-free and continuity of the normal stress at the inner-outer core boundary. For the non-dimensional equations, that

means that we can define a "phase change number" P so that the normal stress at the boundary is -P u_r with the radial velocity u_r. This number characterizes the resistance to phase change at the boundary, with P → 1 corresponding to infinitely slow melting/freezing (or a free slip boundary), and P → 0 corresponding to instantaneous melting/freezing (or a zero normal stress, corresponding to an open boundary). This parameter P, together with the Rayleigh number Ra, controls the style of convection in the inner core. For low Rayleigh numbers there is no convection, and thermal diffusion dominates the heat transport. For higher values of Ra, the style of convection in the inner core depends on P: For high P, convection is dominated by thermal plumes whereas for low values of P, the inner core is in a translation regime, where material freezes at one side and melts at the other side, so that the velocity field is uniform, pointing from the freezing to the melting side.
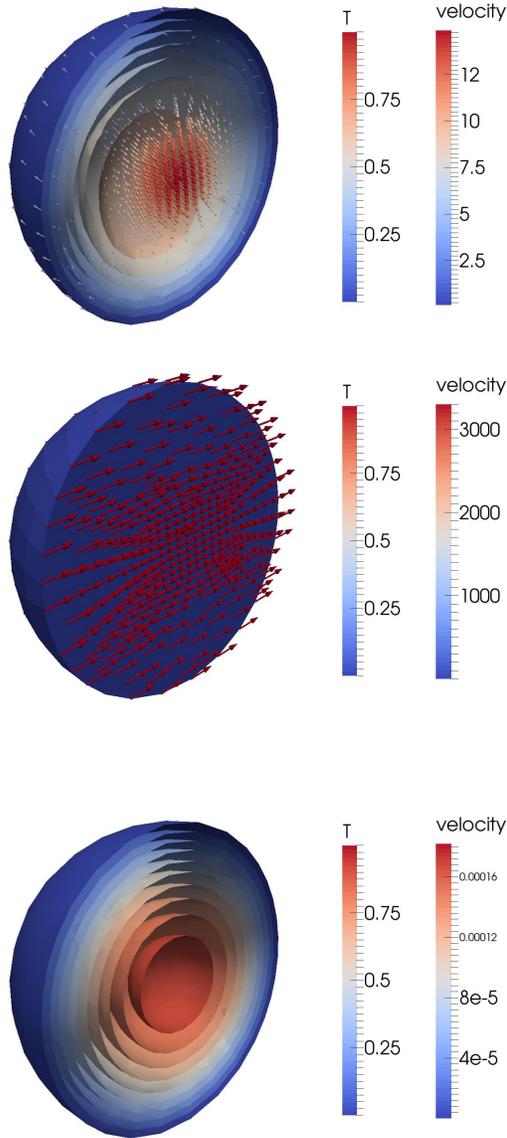
The figures show the different regimes of convection in the inner core for different values of Rayleigh number Ra and resistance to phase change P at the inner/outer core boundary. From top to bottom: plume convection, translation, no convection.

Improvements of the Newton solver

(Menno Fraters)

I made large improvements in debugging the Newton solver, and making it more resilient to material models that create non-Symmetric Positive Definite matrices, by adding a series of tests to the assembly in debug mode. This will make the debugging of material models that implement the derivatives of material properties required for the Newton solver a lot easier. We

also investigated the behavior of the Newton solver, and discussed improvements to the globalisation and prevention of oversolving.

Geoid Postprocessor

(Rene Gassmoeller, Anthony Osei Tutu, Ian Rose, Shangxin Liu)

We worked on improvements of the different geoid postprocessor implementations that were available before the Hackathon and did a first (general) comparison to a spherical harmonics code.

We have implemented several different geoid postprocessors, including both a standard and a multipole implementation. We have worked on generating reference output for benchmarking from HC, CitcomS, and analytic solutions. These reference solutions have been challenging to create and interpret due to uncertainties in scaling choices and significant mesh effects. This project is ongoing.

Attached are geoid maps of our simple test case and a first result for the S40RTS/SAVANI tomography model, computed with Shangxin's implementation. We need to find a better way to further benchmark our codes.

Degree 2 order 2 test case with 2 global refinements

Global Degree 2 Geoid Anomaly with ref 2
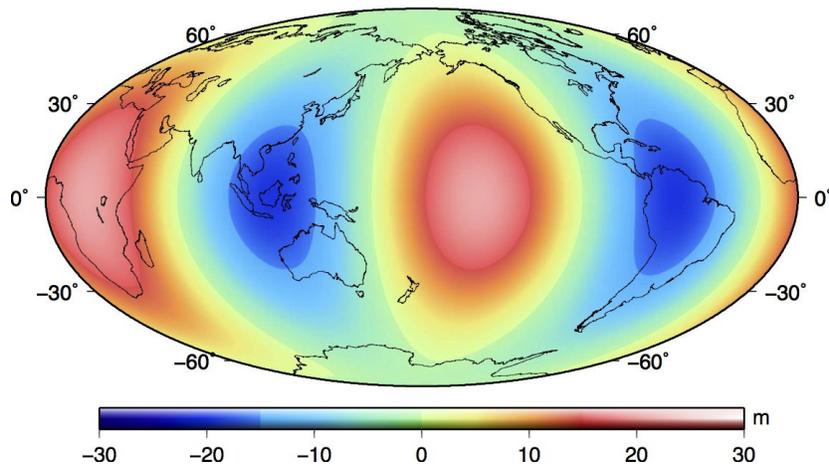
Global Geoid computed from SAVANI (2-60 degree):

SAVANI, Karato scaling, E30
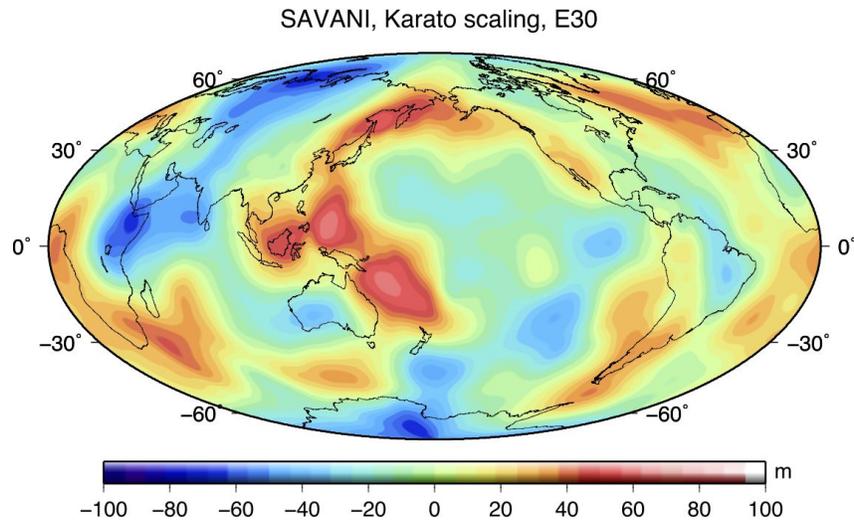
Geoid Benchmarking

(Anthony Osei Tutu)

I worked as part of the geoid postprocessor implementations group on providing a benchmark case using the spherical harmonics code HC to estimate the degree 2 geoid and geoid kernels for the different postprocessors currently available in ASPECT; the multipole and standard method. I also spent time working on the scaling of the standard geoid estimate method that was implemented using the same approach that is used in CitcomS. This is ongoing work, and currently there are significant mesh effects and even at higher degrees, there seems to be a dominance of degree two when we tried using S40RTS as temperature initial condition.

Improvements to tracer particles

(Rene Gassmoeller, Elbridge Gerry Puckett, Harsha Lokavarapu, Cedric Thieulot and many others)

Rene Gassmoeller

I implemented a way to decide for each compositional field in the code whether it should be advected by a field method or by particles (potentially allowing for comparing the two methods, and also allowing to use all particle properties within the computation). Attached is an example figure of a particle field that was interpolated to a cell-wise constant compositional field that may be used in the finite-element computation. Many others (John, Harsha, Gerry, …) used the particles for their purposes (see their sections). I provided data and models to Cedric to allow for the comparison of the divergence of the velocity at the particle positions, and we found that the 'particle clustering' problem many lower order codes have and solve by implementing a CVI

(consistent velocity interpolation) correction term is negligible for higher order elements like the Q2Q1 elements of ASPECT. Attached are figure comparisons for different finite element orders. Note how the edges between the deformed and undeformed domain become increasingly depleted / enriched by particles at lower orders, despite increasing the mesh resolution by a factor of 2 for every decrease of polynomial order.

Q1P0

Q2Q1

Q3Q2

Active
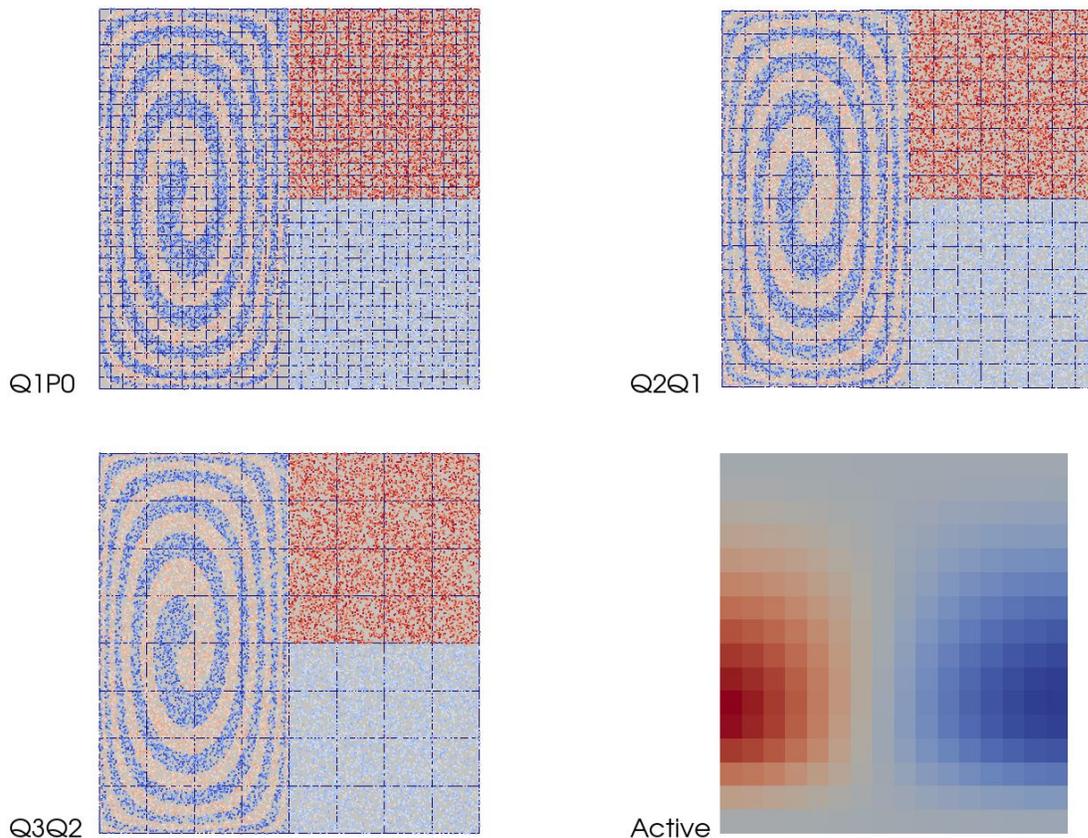
Harsha Lokavarapu

I opened several pull requests that relate to extending the functionality of ASPECT such as outputting particle data in multiple formats, a starting point for a scalable particle generator in a uniform box distribution, and improvements of the checkpoint system. I also worked on a scalable particle generator that solves the placement of particles on edges. This is an effort to further research involving the utilization of particles to understand time scales of mixing properties that are being supervised by Gerry Puckett, and Louise Kellogg.

Elbridge Gerry Puckett

1. I collaborated with Cedric Thieulot and Rene Gassmoeller on the Continuous Velocity Interpolation (CVI) project and paper. This included analyzing the nature of the terms that are added to the velocity components (u,v) to make them divergence free.
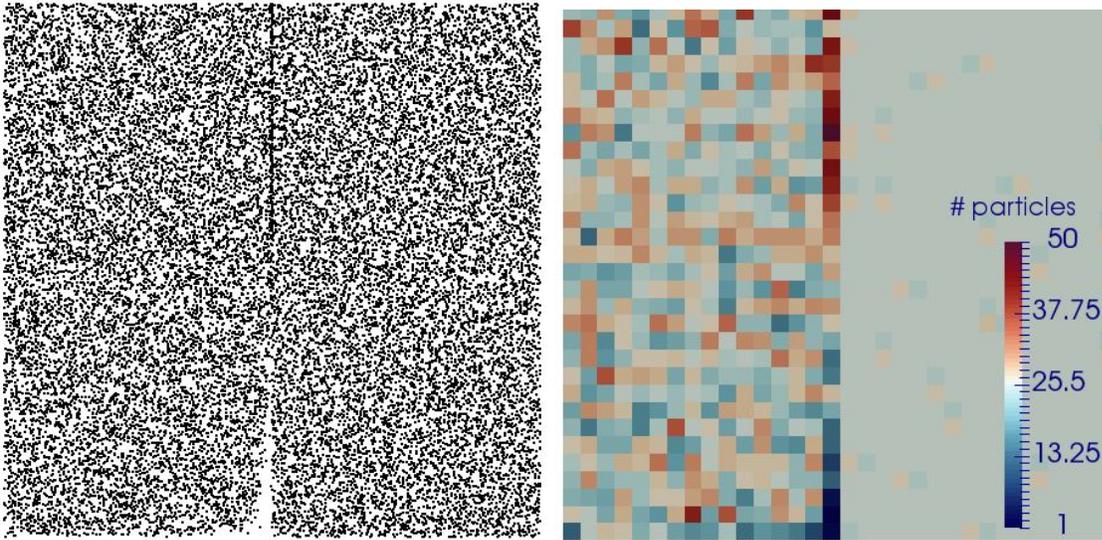
Figure showing the error in the particle positions when the particle velocities are evaluated only with the Q1 elements.
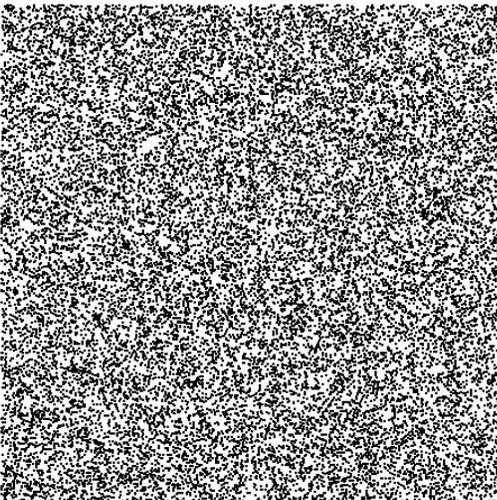
Figure showing the particle positions when the particle velocities are evaluated with a Q2 velocity field in ASPECT.

2. I started a project to examine the convergence rate of the active tracer particle interpolation algorithms. This includes implementing the least squares interpolation algorithm described in M. Thielmann, D. A. May & B. J. P. Kaus, "Discretization errors in the hybrid finite element particle-in-cell method", Pure and Applied Geophysics, 171, 2165–2184, 2014, DOI: 10.1007/s00024-014-0808-9 and conducting the convergence rate studies shown in that paper.

3. I started to work on a 2D Convection Rolls cookbook using the Turcotte stability analysis

example

4. I worked with Harsha Lokavarapu on specifying the functionality that is required of the Binary I/O and the new rotating checkpoint files. (See Harsha's report above.)

Cedric Thieulot

I discussed Conservative Velocity Interpolation (CVI) with Rene and Gerry. We started working on a 'technical note' paper to be submitted to Gcubed, as a response to the paper by Wang et al, Gcubed 2015. This quickly turned into a multi-sided research. I explored many parameters within the linear element based code ELEFANT and compared some of the results with those obtained with ASPECT for a range of elements (Q1P0,Q2Q1,Q2P-1,Q3Q2). I spent the best part of the week running both codes and making plots, writing the paper, and worked (with Gerry among others) on the actual form of the CVI algorithm. Following the small presentation I gave on Friday we started to look into particle spatial distributions, configuration entropy and Lyapunov exponent. I'll continue working on this in the coming weeks and hope to submit the paper at the end of the summer.
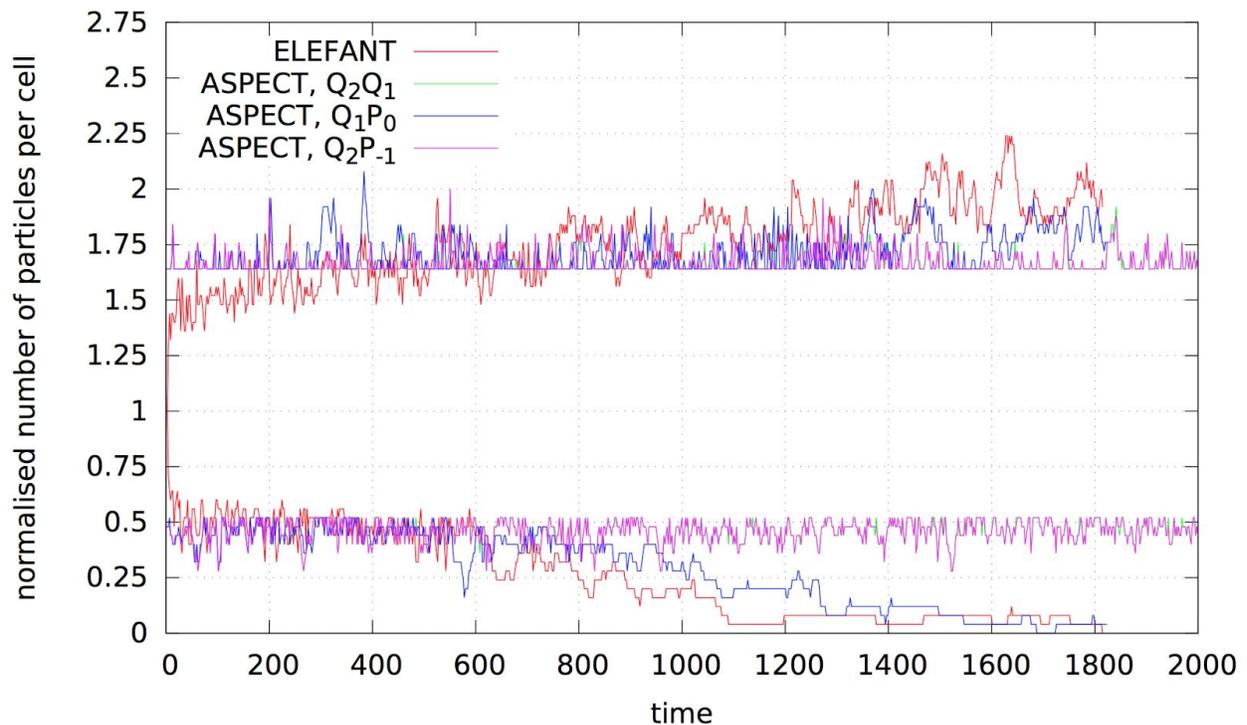

Time evolution of the normalised minimum and maximum value of particle number per element for ELEFANT (red) and ASPECT with Q2Q1 elements (green), with Q1P0 (blue) and with Q2P−1 (purple).

I got the news that the Dutch NSF has granted me 3 years of funding for a postdoc to use ASPECT and carry out detailed whole Earth modeling and look in particular at gravity.

Computing the 1D lithostatic pressure profile

(Anne Glerum)

I added a plugin that calculates a 1D lithostatic pressure profile in a user-specified point that is used to prescribe the normal traction on one or multiple boundaries. This way, material is free to flow through the boundary ("open boundary"). Below a figure of a model with a free surface and an open bottom boundary. Three columns are set of which the middle one is denser and more viscous. The lithostatic pressure is calculated in one of the outer columns and therefore the middle column sinks until it reaches isostasy. The model is included as a test.
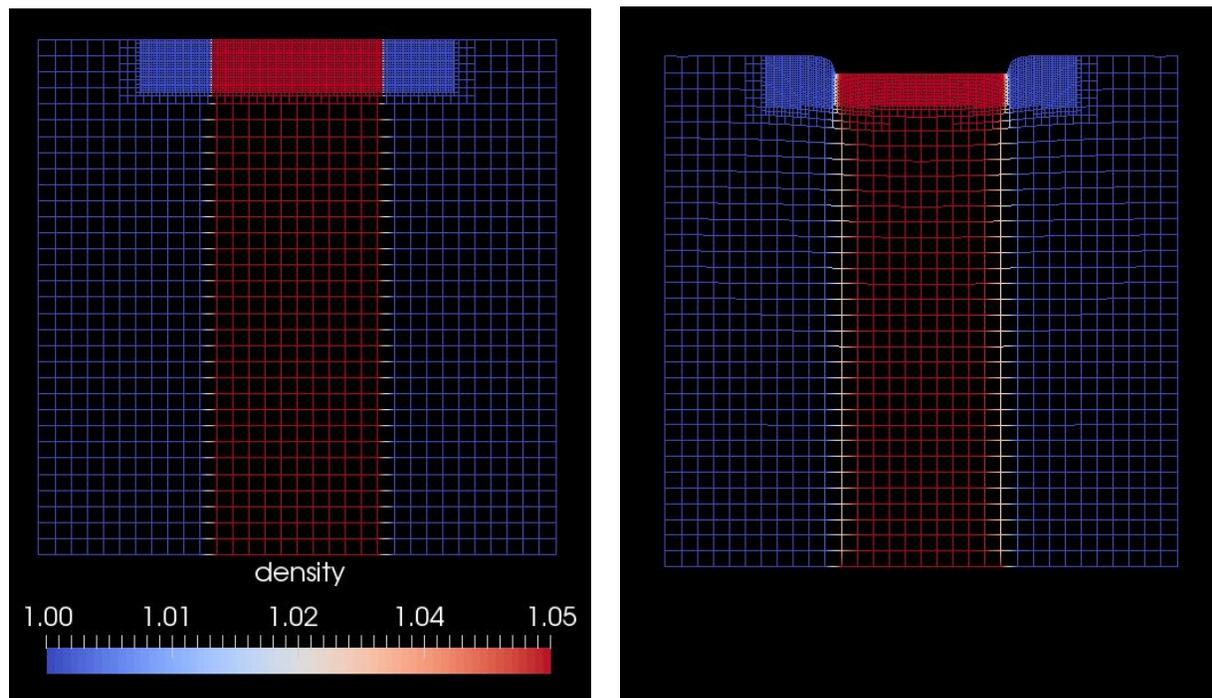
Density and mesh at t0 (left) and t100 (right).

Adding initial topography to the mesh

(Anne Glerum, Menno Fraters)
We set up the framework to add initial topography to the mesh. In addition to the plugin "zero topography", we will add plugins that specify the topography through polygons in the input files as well as from separate data files.

Dynamic Citation Information

(Timo Heister, Lorraine Hwang, Louise Kellogg)

We discussed and decided after a long discussion how we want ASPECT to be cited. We reviewed current thoughts and projects in giving credit for software and how ASPECT should be cited including versioning, and we collaborated on an embedded html solution. An initial implementation of a website that generates citation information based on the computation being done has been made, but not merged. See https://geodynamics.github.io/aspect/cite.html for the current version.

Improvements to the DG bound preserving limiter

(Ying He)

I implemented the 3D DG bound preserving limiter. I did some experiments on how the viscosity harmonic average can affect the convergence of the Stokes solver for advection fields using both FEM and/or DG methods. I also spent a lot time to investigate why the DG approach has a very large memory cost with a longer computation time compared with the FEM approach. We found that the current implementation of the matrix sparsity pattern in deal.II that is used for the DG implementation is not as efficient as the corresponding function call for FEM and plan to improve this efficiency.

Surface processes

(Lev Karatun)

I made a proof-of-concept model for surface processes implementing a hillslope diffusion law, which diffuses/erodes the free surface separately from the motion due to Stokes flow. It will be further used to couple models involving free surface with erosion/deposition. I addition, I added an option ("Adapt by fraction of cells" in .prm files) to switch between refining a certain number of cells based on the fraction of total error (default behavior) and the fraction of number of cells.

Material model with realistic rheologic structure

(Shangxin Liu)

I worked on implementing a realistic Earth-like rheology structure into ASPECT's material model including three parts: weak plate boundary, differences between oceans and continents, and RUM slabs model, as shown in the figures below:

Global viscosity slice surface

Global density anomaly slice surface
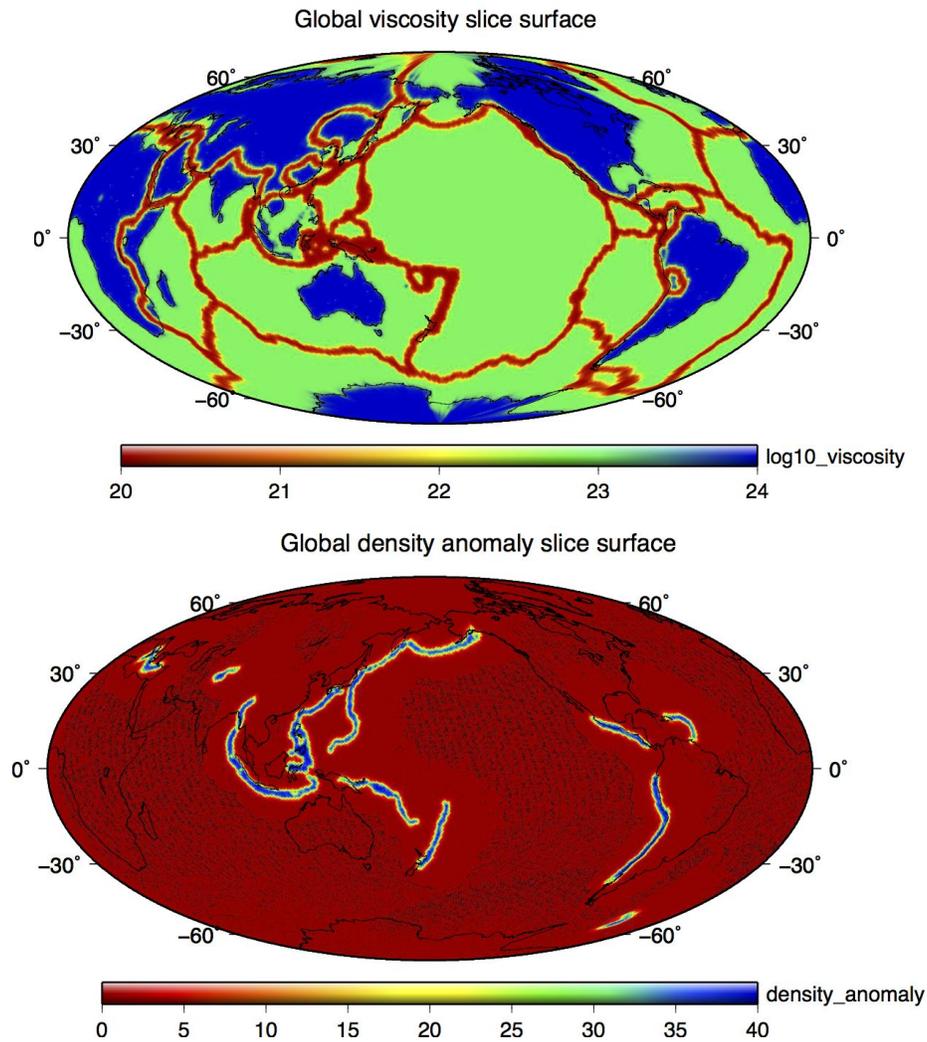
Stress limiter rheology

(John Naliboff)

I made progress on a number of fronts, including implementing and testing a new stress limiter rheological mechanism in an existing material model (merged), testing an experimental continental extension ("long-term tectonic") model with concurrently implemented ASPECT
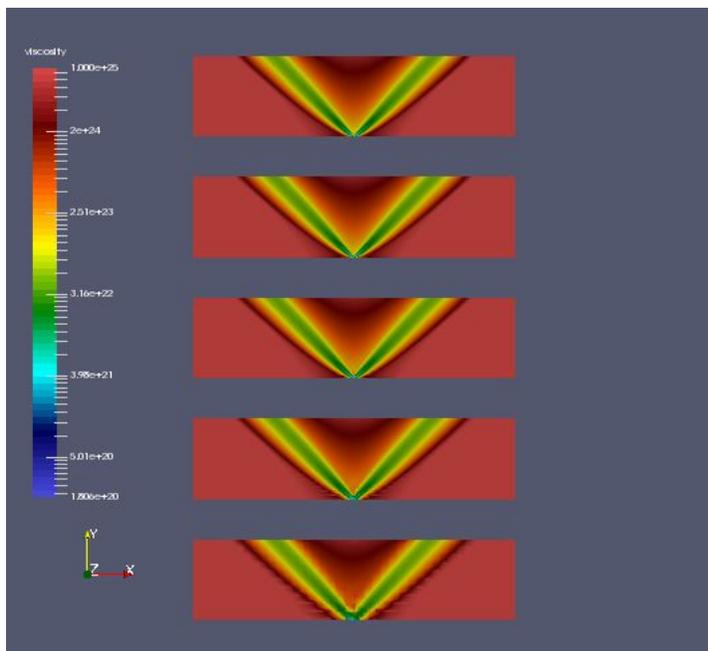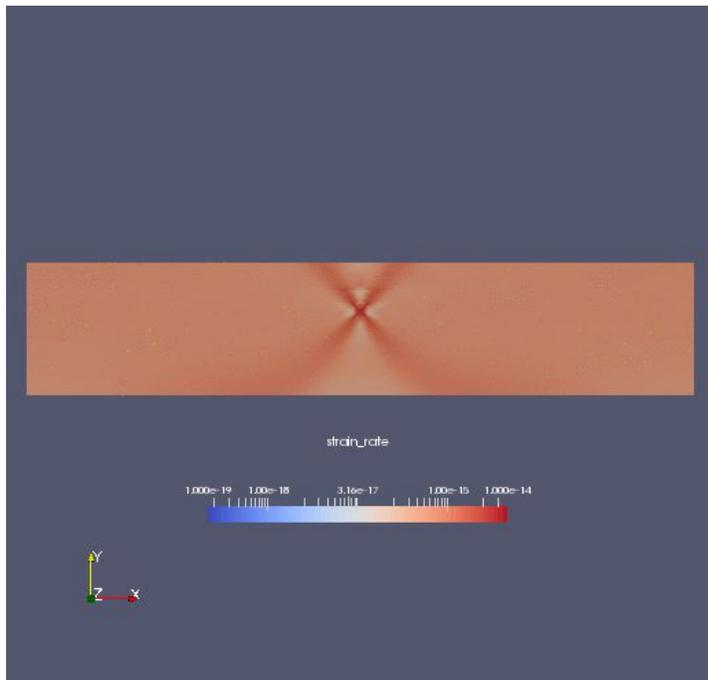
features (DG Limiter - Ying He & Sam Cox; Active Particles - Rene Gassmoeller) and doing preliminary work on implementing Crust 1.0 into ASPECT with Cedric Thieulot. In addition to code development, I also spent a small portion of time researching a method to include an internal length scale within a brittle rheological model. The first figure below shows the results of the implemented stress limiter rheology, which produces resolution-independent shear bands for the given setup. These results match the results produced by Cedric Thieulot with his particle-in-cell code ELEFANT. The second image (animated gif) illustrates deformation patterns (primarily narrow shear bands) within an extending continent (500x100 km) that contains distinct material layers defined by compositional fields. To reduce diffusion along the compositional field boundaries, the computation uses the DG Limiter implementation of Ying He and Sam Cox. Additional simulations are using active tracers (Rene Gassmoeller) in replace of the compositional fields.

VoF interface tracking

(Jon Robey)

I worked on getting the VoF interface tracking closer to being suitable for inclusion and finished basic AMR and MPI support for the VoF interface tracking algorithm.
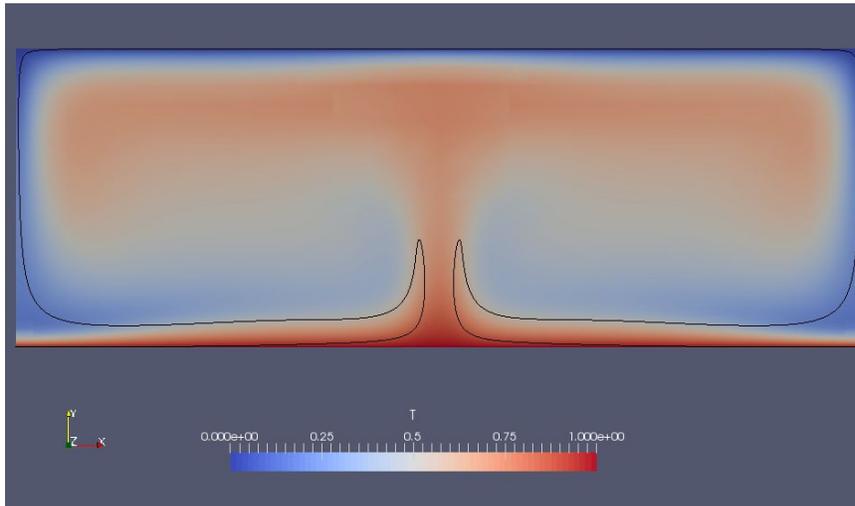

Image of an AMR Convection problem with black contour indicating volume originally in upper boundary layer. Current image is during initial turnover.

Improvements to the free surface

(Ian Rose)

I made significant changes to the internal implementation of the free surface handler. Previously, motion of the surface was handled by moving the vertices of the mesh according to the Stokes velocity solution. Now the mesh motion is handled by keeping a finite element vector that stores displacements from positions in the reference mesh to the computational domain. Performing computations on the real domain involves using this displacement vector with the deal.II mapping MappingQ1Eulerian, which performs the transformation.

The user should see no real changes to computations after this change, but it does make the codebase simpler and easier to maintain. Furthermore, having a mesh displacement vector allows for cleaner interoperation with other features that might modify the mesh. For instance, Anne Glerum and Menno Fraters are implementing a plugin that allows the user to specify initial surface topography which will fit well into this framework. Lev Karatun has made a proof-of-concept model for surface processes implementing a hillslope diffusion law, which diffuses/erodes the free surface separately from the motion due to Stokes flow.

Inclusion benchmark with harmonic averaging

(Benjamin Smith)

I reran the inclusion benchmark with harmonic averaging. As Wolfgang indicated, both velocity and pressure l_2 errors. Results can be found here:

https://docs.google.com/spreadsheets/d/1GYPWl4UOe-Jc5AkVqDX6PDQmL73YU-0S9rwBi7S-Ce0/edit?usp=sharing
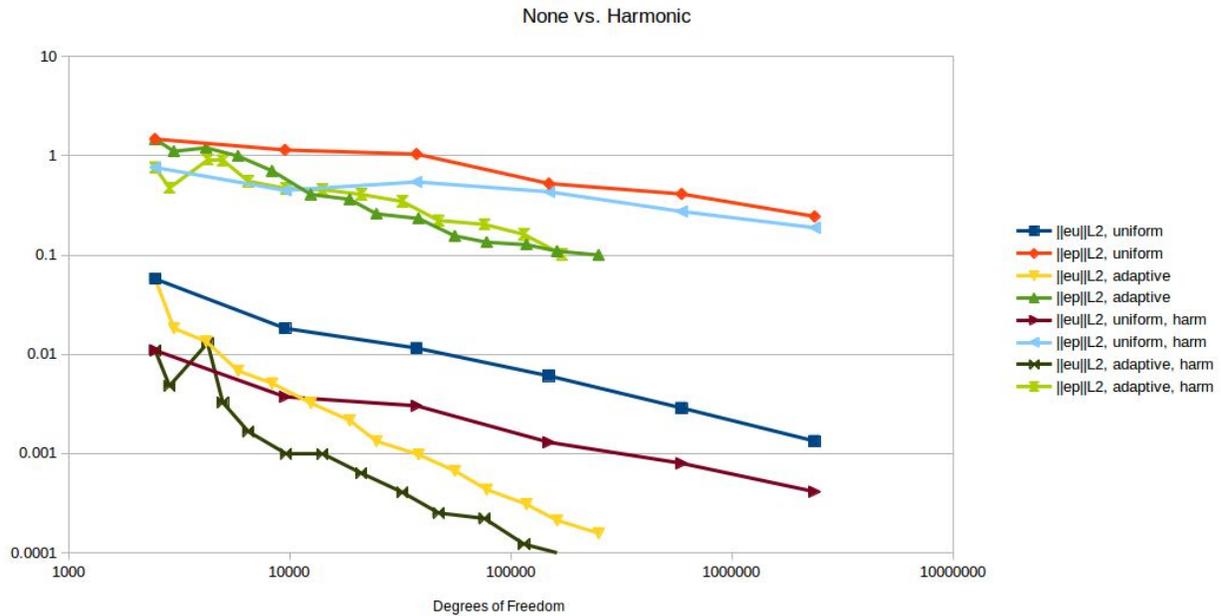
Visualize CRUST1.0 data

(Cedric Thieulot, John Naliboff)

We looked at how CRUST1.0 data are organised and wrote a small program to visualise the data:
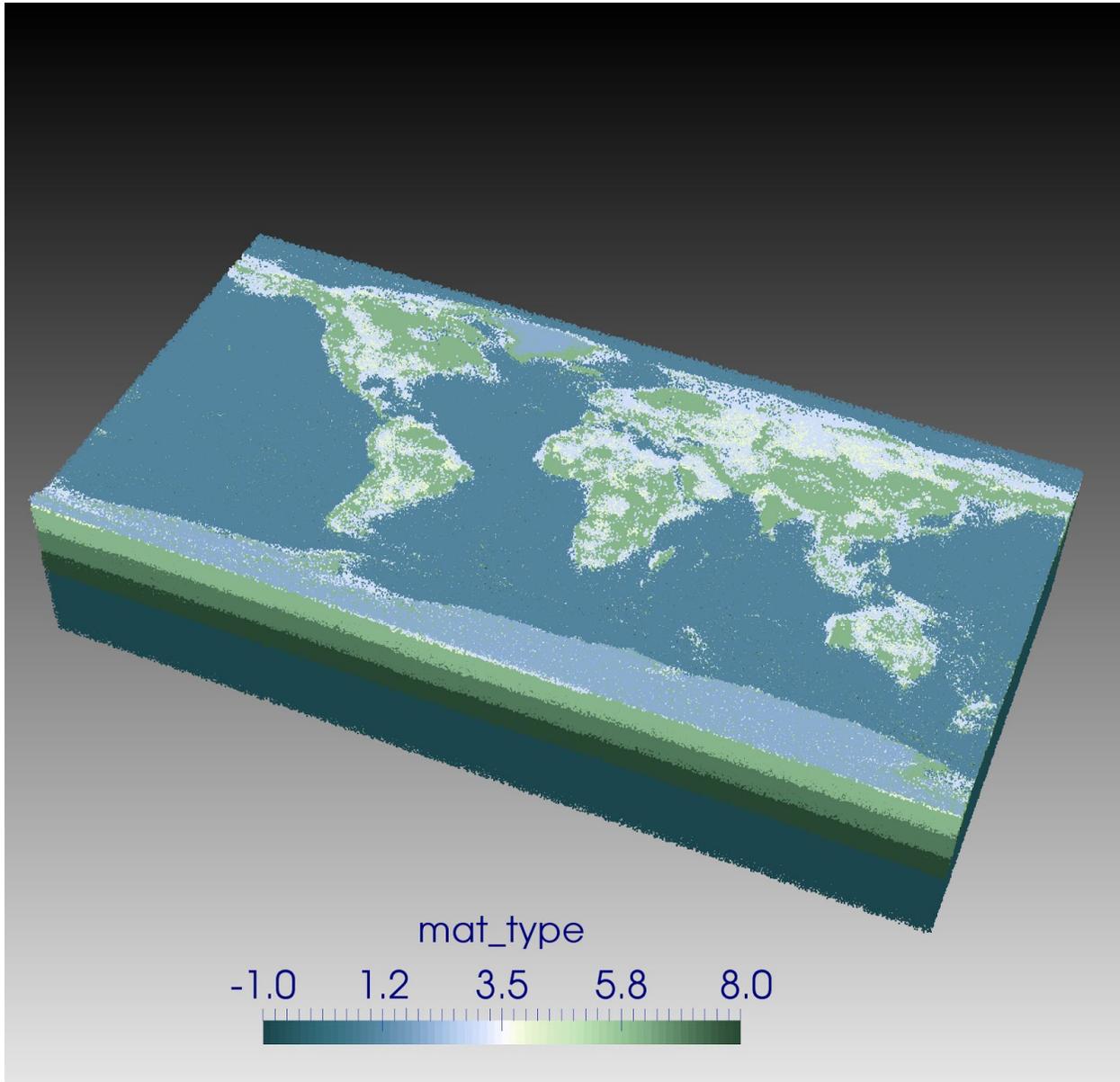
This program will be made part of ASPECT in the summer once the particle interface has been finalised.

Additional contributions

There were a large number of smaller contributions that were merged during the hackathon. The following contains a sample of these:

- Updated the MacOSX installation instructions (Sam Cox)
- Clarified the description of a boundary model (Sam Cox)
- Several updates to fix functionality, for example dG with non-planar faces, and averaging of thermal conductivities (Sam Cox)

- Added Blankenbach benchmark case 2 (Timo Heister, Juliane Dannberg, Cedric Thieulot, Ian Rose)
- Improve cmake project generation (Timo Heister)
- Hide utility solution files inside subfolders in the output directory to improve user experience (Timo Heister)
- Allow tests to have files in subdirectories (Timo Heister)
- fixed the prefactor normalization bug in S40RTS initial condition (Shangxin Liu)
- improved the dynamic topography postprocessor to fix a bug in the average dynamic topography computation and allow the dynamic topography to be computed from the density contrast throughout the top boundary of the domain (Shangxin Liu)
- Added a test for conduction in a spherical shell (Anne Glerum, Ian Rose, Timo Heister)
- worked on the chunk geometry model that was causing velocity singularities (Anne Glerum)
- Added a layered chunk geometry with additional boundary indicators to set multiple boundary conditions on the lateral boundaries (Anne Glerum)
- Discussed the results for last year's software survey and focus groups (Lorraine Hwang)
- Altered most existing benchmark tests to function with MPI (Jon Robey)
- Added and modified code to use multiple small code duplication reduction utilities (Jon Robey)
- Revised logic for lateral average calculation to warn about over-resolution resulting in bands without data and do sensible things as a result, and some dependent material models (Jon Robey)
- Fixed a bug in the S40RTS and SAVANA perturbation implementation files that caused files not to be found if a user-specified data directory did not end in a trailing slash (Benjamin Smith)
- Fixed a bug that caused the program to hang in parallel when processor 0 broadcast a file read error and the other processors never received the broadcast (Benjamin Smith)
- Fixed spelling/grammar in a few places (parameters.cc, S40RTS_perturbation.cc, SAVANI_perturbation.cc) (Benjamin Smith)
- Tested whether it makes a difference in number of iterations/solve time when using the full A term in the preconditioner (results inconclusive) (Benjamin Smith)

Statistics about ASPECT's growth during the hackaton

The following contains a number of statistics about how much ASPECT has grown during the hackton:

- Number of source files in ASPECT before/after: 384 -> 427   +43
- Lines of code in ASPECT before/after: 83,274 -> 91,462   +8,188
- Number of merged pull requests before/after: 663 -> 747   +84
- Commits in github before/after: 3,721 -> 3,957   +236
- Number of tests before/after: 333 -> 380   +47

These statistics were generated through the following commands:
- find include/ source/ | egrep '\.(h|cc)$' | wc -l
- cat `find include/ source/ | egrep '\.(h|cc)$`' | wc -l
- git log --format=oneline | grep "Merge pull request" | wc -l
- git log --format=oneline | grep -v "Merge pull request" | wc -l
- ls -l tests/*prm | wc -l