Global spectral flow code development and benchmark plan

Thorsten Becker
University of Southern California

Active working group:
Thorsten Becker, Clint Conrad, Carolina Lithgow-Bertelloni,
Rick O'Connell, Craig O'Neill, Mark Richards,
Bernhard Steinberger, Shijie Zhong.

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As a result of our discussions (most recently our telecon on 05/15/06), I here summarize the current status and work plan to develop a modular, shared, and well documented global, Hager & O'Connell (1981) type, spectral mantle flow tool. Please keep sending me comments on this document, also if you are not on our mailing list but wish to be kept up to date about progress.

The objective of this project is to provide a commented and well-tested set of modular source codes to allow the user to compute velocities, stresses, and the geoid for a set of different mechanical boundary conditions and spherical harmonics (SH) based density models. Example applications would be testing other numerical implementations (*e.g.* spherical FE codes), teaching, estimating the large scale mantle flow field, and coupling with FE codes, for instance.

Besides the standard viscous-flow solution, we will also strive to incorporate visco-elastic relaxation/transient approaches. There will be an accompanying package to convert from lon/lat data to SH space, and, within a different effort (basically, an update of Becker & Boschi, 2002, as hosted by the European SPICE network), several global tomographic models will be provided for download.

Progress up to May 2006

1. We agreed on benchmarks for cross-code comparison and comparison with analytical solutions. Those benchmarks are specified in this document below. Benchmark results are available from Bernhard's code (complete), and the new HC derivative of it (only velocities). Results match, but there's the well known problem with numerical instabilities for density expansion with high spherical harmonic degree.
2. We still collect existing, working codes (Bernhard, Carolina, and Mark agreed to share

their routines). We work to make those easily compilable, in effect establishing a repository for existing codes. If possible, run benchmarks with existing codes before sharing them with instructions how to do so. We have gotten Bernhard's code.

3. As of our telecon in mid May, we decided to go ahead with Thorsten's HC rewrite of Bernhard's code. This code is to form the basis of the new community tool.
   The code is available for download right now in a pre-release state at the CIG subversion repository http://www.geodynamics.org/websvn/ in the subdirectory /mc/3D/hc, It is functional for velocity computations only, but can run all benchmark tests using a script and input files also found in the repository.
4. The working version of HC flow code has a modular spherical harmonics implementation and is purely written in C. Functionality:
   a) Free-slip, no-slip, and plate (SH expansion) surface mechanical boundary conditions.
   b) Only radial viscosity variations with an arbitrary number of constant viscosity layers.
   c) Compute incompressible viscous flow solution without phase boundaries and constant gravity throughout mantle robustly up to spherical harmonic degree of 50 or 100.
   d) Density model can be input as SH parameterization (*e.g.* using Thorsten's, Dahlen & Tromp normalization, format).
   e) Output of velocities.
   f) Planned functionality for the near future (before first “official” release):
      i. Compute stresses
      ii. Compute geoid

5. Document and match analytical as well as cross-code benchmark solutions (see appendix). Within a makefile “test” directory, allow the user to compute both analytical benchmark solutions and run Bernhard's, Mark's and the new code for comparison with each other. Formulate benchmarks such that CitcomS solutions can be computed and compared with as well. Benchmarks are eight selected cases as documented in the appendix.
   The HC directory of the subversion server at CIG holds scripts to run these tests with the HC code, and Thorsten has results from Bernhard for all tests. HC and Bernhard's original produce matching velocity solutions (as they should).
6. Provide a complete description/writeup of the theoretical approach within a README type document (many of the published papers contain known typos in the equations). Write results up in a technical paper for publication in G-Cubed.

Planned later extensions:

1. Implement compressibility and phase transitions following Panasyuk *et al.'s* (1996) or Steinberger's approach;
2. Along the line of 1., adjust the depth dependence of *g* include self-consistent gravitation, or density from PREM.
3. Implement visco-elastic relaxation solution (Love numbers).
4. Provide an external set of routines to solve for rigid plate motions following Ricard & Vigny (1989) following Carolina's or Bernhard's implementation.
5. Implement the iterative solution method for flow in the presence of lateral viscosity contrasts. Implement Steinberger *et al.* (2001) solution for stresses in the lithosphere (as a thin sheet).

Personnel involvement:

Bernhard Steinberger: Contribute flow code with extensions, run benchmarking.

Carolina Lithgow-Bertelloni: Contribute flow code, contribute analytical solutions, theory descriptions and benchmarks.

CIG: Provides subversion repository and collaboration support. Planned collaboration on flexible spatial representation of data on sphere.

Clint Conrad: Assist in benchmarking of flow codes and CitcomS comparisons.

Craig O'Neill: Expand HC community code, run benchmarks, lead in writing paper on project efforts.

Mark Richards: Contribute flow code, discuss implementation strategy for visco-elastic relaxation problem with Jerry Mitrovica, assist in benchmarking.

Rick O'Connell: Check/implement a more robust propagator/two point boundary value approach. Assemble benchmark solutions and theory write-ups.

Shijie Zhong: Liaison with CIG for potential repository and programming support.

Thorsten Becker: Set up benchmark testing suite. Continue to rewrite Bernhard's code in a modular, pure C way (HC code). Implement geoid computation.

Appendix: Benchmark parameters

In the following, we list three boundary conditions, three viscosity structures, and four density structures, making for 36 potential test cases. We suggest to focus on free slip/no slip, viscosities 3a) and 3b), and density structures 4a), and 4c), making for eight initial test cases.

If all test cases are run, we suggest the following **naming convention for subdirectories**: Call the directories "out**ijk**", where **i = a, b, c** for the mechanical surface boundary conditions (free slip, no slip, plates). Parameter **j** is for viscosity structures **a, b,** and **c** (see below), and parameter **k = 0, a, b, c** is for the density models d0 (Shijie's test), and d1 through d3, respectively.

The input files are available through the links given below, and a complete set of input files with a script to run the HC code can be found on the subversion repository at CIG, under http://www.geodynamics.org/websvn/ in the subdirectory /mc/3D/hc, which also holds the HC code.

1. Parameters

In general, use SI units, but cm/yr for velocities, MPa for stresses, and % for density anomalies. For spherical harmonics scalars and poloidal/toroidal fields, use Dahlen & Tromp (1988, B.8) theoretical physics convention or describe how to convert to that format.

Parameter	***Value***
reference viscosity η_0	10^{21} Pas
radius of Earth, R	6371 km
gravitational constant, G	$6.6742\ 10^{-11}$ N m^2/kg^2
gravitational acceleration (constant throughout Earth for simplicity, incompressible computation), g	10 m/s^2
seconds per year, *spyr*	31556926
average mantle density (constant), ρ_m	4448.8 kg/m^3
core density (relevant for jump across CMB, and made to be consistent with ρ_m and g), ρ_c	11601.01 kg/m^3
radius of core, R_c	3480 km ($r = R_c/R = 0.546225$)
thickness of mantle, T_m	2891 km

2. Boundary conditions (i – parameter in out*ijk* convention)

CMB is free slip, surface is at least free-slip (**a**), or no-slip **(b)**. To test toroidal flow solver part, also try to compute velocity and geoid solutions with prescribed surface velocities (**c**). For plates, use NUVEL-HS2 in NNR reference frame, expanded without tapering up to spherical harmonic degree 127 at
http://geodynamics.usc.edu/~becker/ftp/flow_bench/nnr.nuvel.127.pt.ab.gz
in units of cm/yr and Dahlen & Tromp (1998) format, listed in
A_{lm} B_{lm} C_{lm} D_{lm}
where A, B are poloidal, and C, D toroidal flow components (see, *e.g.*, http://geodynamics.usc.edu/~becker/tomography/node12.html)

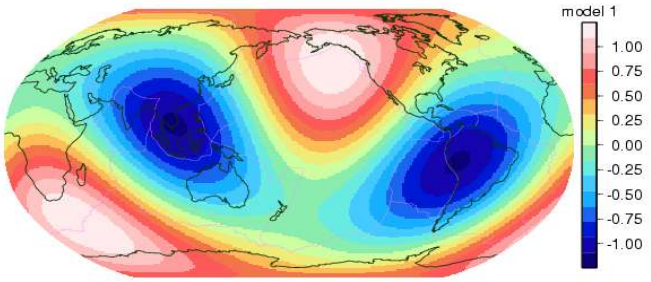
3. Viscosity structures (j parameter in out*ijk* convention)

a) constant throughout mantle at reference value 1 (times reference viscosity)
b) Upper 100 km (<= 100km) and lower mantle (> 660km) 100, upper mantle 1 times reference viscosity.
c) 14 layers as specified in the file at http://geodynamics.usc.edu/~becker/ftp/flow_bench/visco.b3
Format: first line: nd # of data entries. Following nd lines: R/R_{earth} η/η_{ref}
where every entry marks the viscosity of the layer that is terminated by R at the top.

4. Density structures (k parameter in out*ijk*)

All discrete models are given as spherical harmonics expansions in Dahlen & Tromp (1998) convention on 58 evenly, 50 km spaced layers from 2870 km to 20 km depth throughout the mantle using the file format convention as described on
http://geodynamics.usc.edu/~becker/tomography/node12.html
The densities are all given in percent of a constant density (as the code is supposed to be incompressible).
The test models are available for download and are given by:

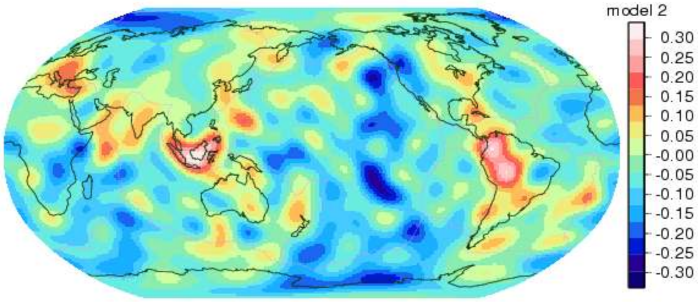
0) Zhong *et al.*'s (2000) first appendix C1 benchmark with a single layer at mid mantle depth. Only for this test, use Shijie's viscosity structures and inner core radius of $R(\text{core})/R(\text{earth}) = 0.55$ instead of 0.546225. More specifically (paraphrased from Shijie's comments, equation numbers refer to Zhong *et al.*, 2000): The equations that were solved were the non-dimensional conservation equations (*i.e.*



eqs. 6 & 7) where the driving force is represented by $X\,Ra\,T$, where X and Ra are defined in eq. 9. For this benchmark, T is given in equation C1 (*i.e.*, a delta function in radial position at the mid-mantle depth multiplied with a spherical harmonic function of some l and m), and $X\,Ra = 1$. This use of a delta function here is similar to those in kernel calculations by Richards and Hager (1984) and Hager and Richards (1989). If you use density in eq. 2, then $X\,Ra\,T$ is $d\rho\, g$. Notes: (I) On the implementation of the delta function in the analytic solution and in the finite element method: For the analytics, the delta function in radial direction really simplifies the solutions (Hager and O'Connell, 1981, talked about this). For finite elements, we let T be zero everywhere except on one layer of nodes (*i.e.*, at r=(ro+ri)/2 or mid-mantle) where T is equal to (1/dr)*Y(l,m), where dr is the radial grid spacing or (ro-ri)/nel_r with nel_r as the number of element in radial direction. (II) There might be a minor error in the description of this benchmark in appendix C of Zhong *et* al. (2000), where it is stated that $Ra=1$ not $X\,Ra=1$ as stated above because of technical changes in the revisions.

a) A degree 2 pattern whose amplitude oscillates with two sine functions throughout the mantle. The density anomaly is shown below at 1020 km depth, units are %, and the coefficients are available at http://geodynamics.usc.edu/~becker/ftp/flow_bench/d1.m.ab.gz

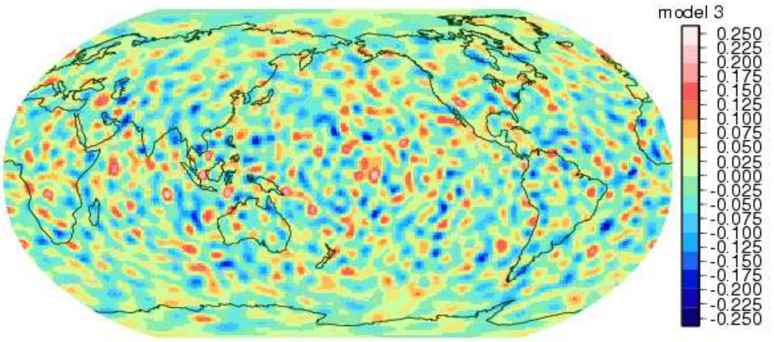
b) The 3rd model is Ritsema and van Heijst (2000) S20RTS seismic tomography model scaled by 0.2, re-parameterized and interpolated to the same depth levels as model 1. (Don't further scale this model, it is already in given in density anomalies in percent.) At 1020 km, this model should look like so:



and the coefficients are at http://geodynamics.usc.edu/~becker/ftp/flow_bench/d2.m.ab.gz

c) The 4th model uses a random, white noise spectrum, looks like plotted below at

1020 km, and can be downloaded at
http://geodynamics.usc.edu/~becker/ftp/flow_bench/d3.m.ab.gz



4. Model evaluation

a) Evaluate velocities at surface, CMB, and 1020 km depth in spherical harmonics for the three density cases, all formally up to degree and order 50, Dahlen & Tromp (1998) poloidal/toroidal format. Evaluate velocities at same depth on 1 by 1 degree grid going from 0 to 359 lon, and -89.5 to 89.5 latitude.

b) Evaluate geoid kernels, and surface geoid in meters, spherical harmonics. For the geoid, assume an incompressible core and mantle and use a constant gravity of 10 m/s^2 for simplicity.

c) If code allows for it, evaluate stresses τ_{rr}, $\tau_{r\theta}$, $\tau_{r\phi}$, $\tau_{\theta\theta}$, $\tau_{\theta\phi}$, $\tau_{\phi\phi}$ in MPa at same layers, where r, θ, ϕ are the regular spherical coordinates radius (unit vector up), co-latitude (unit vector South), and longitude (unit vector East).

5. References cited

Becker, T. W. and Boschi, L.: A comparison of tomographic and geodynamic mantle models, *Geochem., Geophys., Geosys.*, **3**, 2001GC000168, 2002.

Dahlen, F.A., and Tromp, J., 1998, *Theoretical Global Seismology* , pp. 1025, Princeton University Press.

Hager, B.H. and O'Connell, R. J. A simple global model of plate dynamics and mantle convection, J. Geophys. Res. 86, 4843-4867, 1981.

Hager, B. H. and M. A. Richards, Long-wavelength variations in Earth's geoid: Physical models and dynamical implications, Phil. Trans. R. Soc. Lond., A 328, 209-327, 1989.

Panasyuk, S. V. and Hager, B. H, Forte, A.M., Understanding the effects of mantle compressibility on geoid kernels, *Geophys.J. Int.*, 124, 121-133, 1996.

Ricard, Y., and C. Vigny. Mantle dynamics with induced plate tectonics. Geophys. Res., 94, 17543-17559, 1989.

Richards, M. A., and B. H. Hager, 1984, Geoid anomalies in a dynamic Earth, J. Geophys. Res., 89, 5987-6002.

Ritsema, J. and H. J. van Heijst, Seismic imaging of structural heterogeneity in Earth's mantle: Evidence for large-scale mantle flow, *Science Progress*, 83, 243-259, 2000.

Steinberger, B., H. Schmeling and G. Marquart (2001). Large-scale lithospheric stress field and topography induced by global mantle circulation, Earth Planet. Sci. Lett.186, 75-91.

Zhong, S., M. T. Zuber, L. Moresi, and M. Gurnis, Role of temperature-dependent viscosity and surface plates in spherical shell models of mantle convection, J. Geophys. Res., 105, 11063-11082, 2000.