

Cider Practical 2016 - Composition of the Lower Mantle

using BurnMan (thermoelastic property toolkit)

and Mineos (computation of Earth's normal modes)

Sanne Cottaar & Jessica Irving

Global geophysicists have an ongoing discussion on the degree of whole-mantle convection versus the degree of two-layered convection. There is good certainty that in the present day there is exchange of some material between the upper and lower mantle in the form of downgoing slabs and upgoing mantle plumes. Questions which remain are whether this has always been the case and if this material exchange has been sufficient to create a well-mixed mantle. One way to assess these questions is to test if the upper and lower mantles have similar compositions. For the upper mantle we have more direct samples from volcanoes and mid-ocean ridges. For the lower mantle we can attempt to determine the composition based on seismic velocity models.

BurnMan is an open source Python toolkit that computes thermoelastic properties using an equation-of-state for composites at high pressures and temperatures. The equation-of-state parameters come from databases compiled from many experiments of minerals under high-(P,T) conditions. The code provides the tools to directly compare the computed velocities to seismically observed ones. BurnMan is the result of a CIDER 2012 working group. BurnMan was the code we used in Tuesday's tutorial, so we hope that you will continue to get more comfortable working with it today.

Mineos is a venerable open source code in Fortran that calculates the eigenfrequencies and eigenfunctions (and synthetic seismograms) for 1D seismic velocity and density models. We will stick to the eigenfrequencies here and compare them to observed eigenfrequencies. Both the BurnMan and Mineos codes are hosted by the Computational Institute for Geodynamics (www.geodynamics.org).

The eigenfrequency data ($f < 10\text{mHz}$) here are all taken from the Reference Earth Model (REM) webpage (<http://igppweb.ucsd.edu/~gabi/rem.dir/surface/rem.surf.html>) and therefore do not contain every recent observation made, but the observations have been provided by a number of groups. Note that we will compare the REM data with spherical, non-rotating, no-cross-coupling estimates for 1D Earth models. For details and references see `data.readme`.

Update the practical files

There are some updated practical files, so first you will need to pull these onto your virtual machine. This is similar but slightly different to the steps you carried out on Tuesday during Mineral Physics Tutorial 1. To update the program and data files go into the directory `burnman_cider2016`, (by typing `cd burnman_cider2016`) and type:

```
git pull origin master
```

Run through the initial setup

Let's first have a look at the radial seismic velocity and density models of the lower mantle. Run step 1 by typing:

```
python lowermantle_fitting_absolute_velocities_1D.py step1
```

This should plot the 1D models available in BurnMan.. Do keep in mind that these are averaged models and the lateral variations in velocity in the lower mantle are larger than the variation between these models.

We will now test two different compositional models for the lower mantle. The pyrolitic model represents a composition similar to the upper mantle (ignoring Ca and Al):

- Pyrolitic model
 - 75% perovskite or bridgemanite (Mg, Fe)SiO₃ with 94% Mg and 6% Fe
 - 18% ferropericlase (Mg,Fe)O with 80% Mg and 20%Fe
 - 7% Ca-perovskite CaSiO₃

The chondritic model is a competing model that suggests the composition the lower mantle should have if composition of the bulk Earth is represented by chondritic meteorites. In this case the lower mantle is enriched in Si relative to the upper mantle.

- Chondritic model
 - 88% perovskite or bridgemanite (Mg, Fe)SiO₃ with 94% Mg and 6% Fe
 - 5% ferropericlase (Mg,Fe)O with 80% Mg and 20%Fe
 - 7% Ca-perovskite CaSiO₃

Run step 2 by typing:

```
python lowermantle_fitting_absolute_velocities_1D.py step2
```

Observe which model fits the 1D model for Vs, Vp and rho best.

Now, it is time to compute synthetic eigenfrequencies, quality factors (the Q values for each mode) and eigenfunctions. And if all went well, step2 has already produced the required input files, named mineos_pyrolite.txt and mineos_chondrite.txt. In these files the lower mantle velocities and density from the prem_noocean.txt have been replaced by the values computed by BurnMan.

Run Mineos by typing:

```
./RunMantles.sh prem_noocean
./RunMantles.sh pyrolite
./RunMantles.sh chondrite
```

This should produce a number of output files and directories, but most usefully *_R.out, *_S.out and *_T.out files for the pyrolitic and chondritic lower mantles as well as for PREM.

Now we can plot the results against the observed eigenfrequencies. There are several choices to be made.

- First argument: Type of plot, choose from 'dispersion_curve', 'quality_factor', 'compare_with_data'
- Second argument: Choose modes to look at 'S' (spheroidal), 'T' (toroidal), 'R' (radial)
- Third and other arguments: model names to be plotted, e.g. 'prem_noocean' (output files from mineos need to be present in the directory, e.g. prem_noocean_R.out).

For example:

```
python plot_normal_modes.py compare_with_data S pyrolite
prem_noocean
```

Hopefully that produced an epic plot. Note that the misfit increases with increasing overtone, as they get more and more sensitive to the lower mantle.

There are lots of things to play around with. Some suggestions are given below. We don't expect you to do all the exercises in the given time frame; you might just like to choose one or two based on your interests.

Option 1. Improve lower mantle composition

Can you do better than pyrolite? Can you find 'premite'? And does it improve the fit the observed eigenfrequencies?

Copy the rock pyrolite and give it a new name. Implement the lines to compute thermo-elastic values for the new rock and plot the results. This way, one can make changes to the new rock, and compare the new values to the original pyrolite. Ways to change the rock (not all of these lead to a 'realistic' rock):

- Change the ratio of perovskite to periclase.
- Change the amount of Fe (and or Al) in the minerals.
- Currently the temperatures are chosen to be the adiabat for pyrolite. You might want to calculate these for a new rock and vary T_0 , or test the Brown & Shankland adiabat. See [burnman-0.9.0/examples/example_geotherms.py](#)
- Implement your own mineral and try to make it fit PREM. See [burnman-0.9.0/examples/example_user_input_material.py](#)

After you find a model that looks like it gives velocities closer to the 1D models, compute the eigenfrequencies, and see if you have improved those.

Option 2. Explore lateral variations in velocity

Run the following to see >10.000 equally spaced S-wave profiles for the tomographic model of French and Romanowicz (2015):

```
python lowermantle_fitting_velocity_variations.py step1
```

In the next step velocities are computed and plotted for different temperatures and iron contents to illustrate the trade-off.

`python lowermantle_fitting_velocity_variations.py step2`

- There are better ways to plot the trade-off. For example plotting velocities for one depth in a composition-temperature space.
- Modify the code to explore the trade-offs for P-wave velocity and density. What 3D parameters need to be constrained in the lower mantle to answer what the cause is of lateral variations?
- Explore the trade-offs with other compositional variations (ratio perovskite/periclase, amount of Ca, iron fractionation across perovskite and periclase).

Option 3. Sensitivity of different modes to Vs and Vp

- Change the input lower mantle composition to fit the S wave velocity (and maybe not the P wave velocity), for example by changing the ratio of perovskite to periclase, and look at the effect compared to observed radial and toroidal modes (as P and S waves fit PREM better). Within `plot_normal_modes.py` you can change the `nmin`, `nmax` and `lmax` of your plot.
- Do the same by fitting the P wave velocity and ignoring the rest. What is the effect on the different modes?

Option 4. Investigate the different eigenfunctions (for the normal mode connoisseur)

We've been looking at the eigenfrequencies and quality factors for these modes, but we've also calculated the eigenfunctions, which you will remember from Miaki Ishii's lecture. You can look at the different eigenfunctions for the modes which are in the files `Eigen_X_model_ASC/S.00000nn.00000ll.ASC` where X is R, S or T, model is chondrite, pyrolite or `prem_noocean` (or your own new model name) and nn and ll are the radial and angular orders for the mode in question. The top line is a header line, then subsequent lines contain depth and the eigenfunctions (either U and V, or U, or W) and their derivatives for that mode. Plot with your favourite plotting routine, and look for any differences. Which sorts of modes show changes in eigenfunctions, and which are virtually unchanged?

References:

- S. Cottaar, T. Heister, I. Rose, and C. Unterborn (2014), BurnMan: A lower mantle mineral physics toolkit, *Geochem. Geophys. Geosyst.*, 15, 1164–1179. Code available at <https://geodynamics.org/cig/software/burnman/>
- S. French and B. Romanowicz (2015), Broad plumes rooted at the base of the Earth's mantle beneath major hotspots, *Nature* 525(7567) 95-99.

- G. Masters, M. Barmine, and S. Kientz (2014). Mineos. California Institute of Technology, Pasadena, CA. Code available at <https://geodynamics.org/cig/software/mineos/>
- L. Stixrude, C. Lithgow-Bertelloni (2011) Thermodynamics of mantle minerals-II. Phase equilibria, *Geophysical Journal International* 184.3 (2011): 1180-1213.