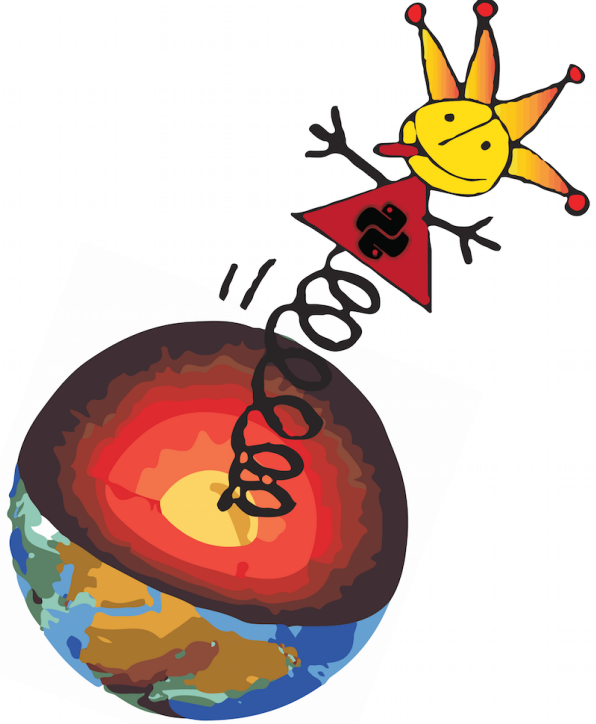


# BurnMan

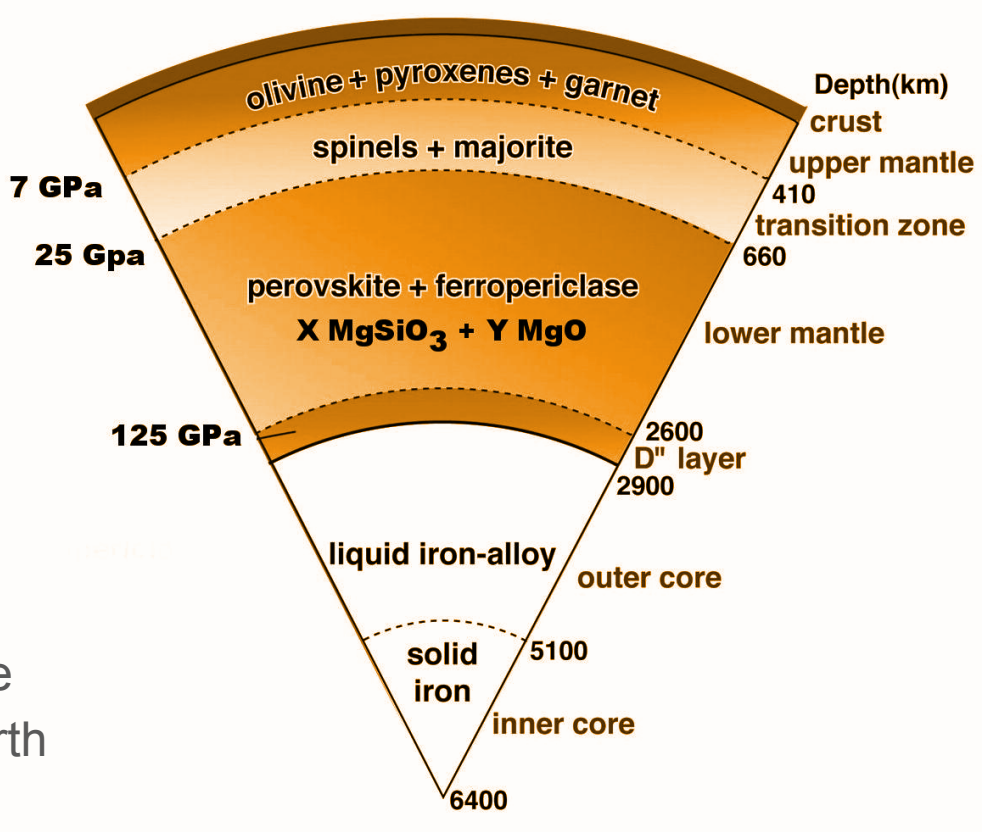
CIG webinar
Oct 8th 2015

Sanne Cottaar, Timo Heister, Bob Myhill, Ian Rose, Cayman Unterborn
https://geodynamics.org/cig/software/burnman/

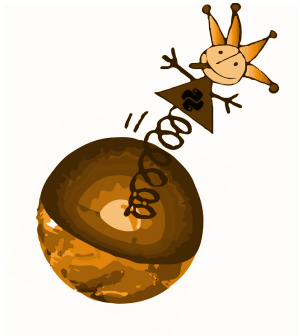
# Introduction

- What is BurnMan?
  - Python library + examples
  - open source
  - modular
  - easy scripts (no user interface)
  - thermoelastic toolkit

- GOAL: Self-consistently compute the mineral properties for the Earth (and other planets)



# History of BurnMan

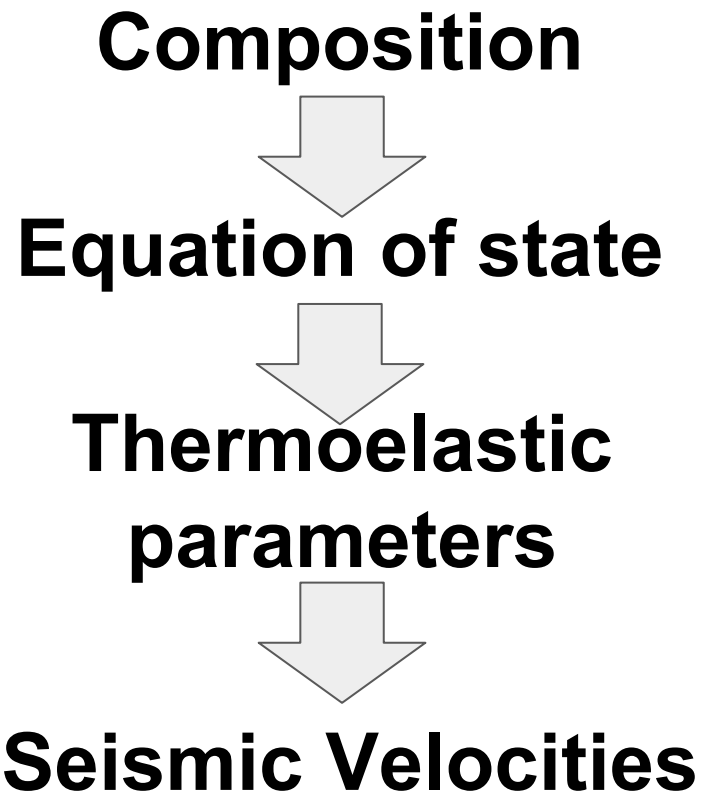


CIDER

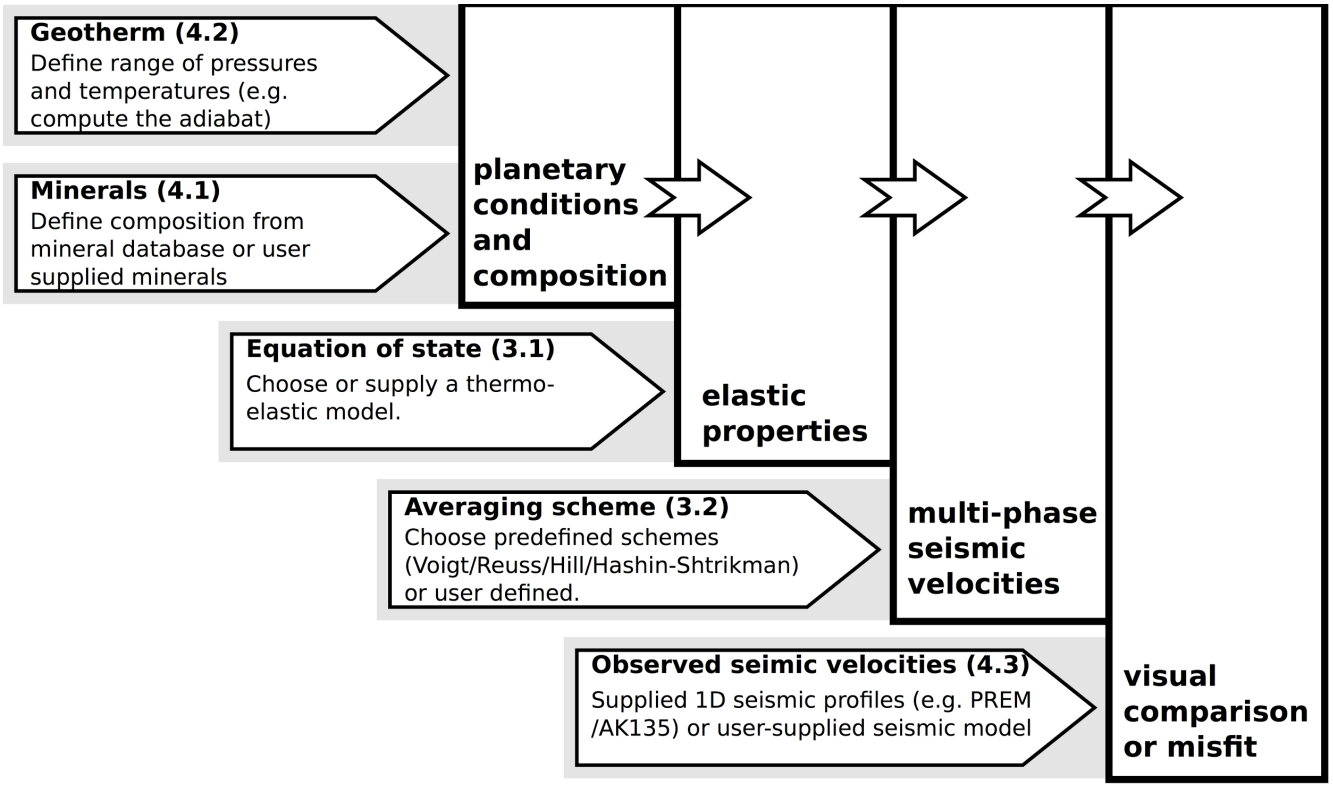
Cooperative Institute for Dynamic Earth Research

- Initial question at CIDER 2012 workshop: ‘What is the Mg/Si ratio of the lower mantle?’ or ‘Do the upper and lower mantle have the same major element composition?’
- Started diving into the forward model - from a composition to seismic velocities.
- Realized that:
  - It is often hard to reproduce the results of a paper.
  - Many people do the same problem with various different codes and excel sheets.
- Started to produce an open source code to improve reproducibility.

# Toolbox overview

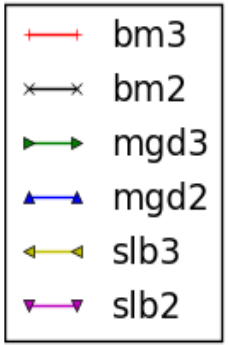


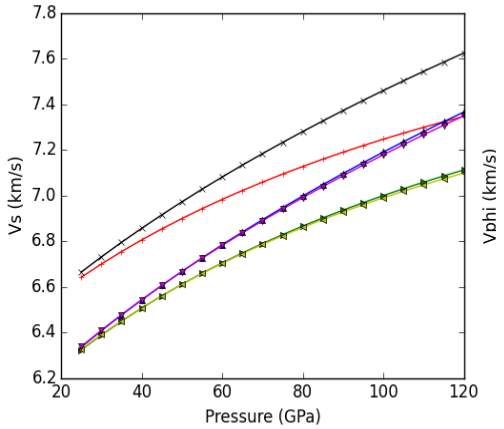
# Detailed Overview



# Equations of state

$$\rho = f(P,T,\boldsymbol{X})$$



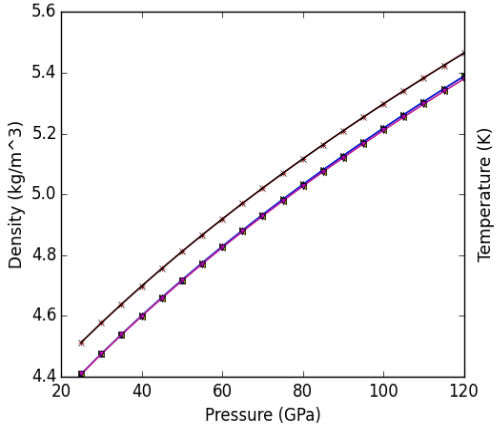




Isothermal EoS:

- Birch-Murnaghan (2nd and 3rd order)
- Modified Tait (Holland & Powell, 2011)

Full thermal EoS:

- Birch-Murnaghan with a Mie-Gruneisen-Debye thermal part
- Stixrude and Lithgow-Bertelloni variant of the same
- Holland and Powell (2001) extension of the Modified Tait




examples/example_compare_all_methods.py

# Equations of state: the bigger picture

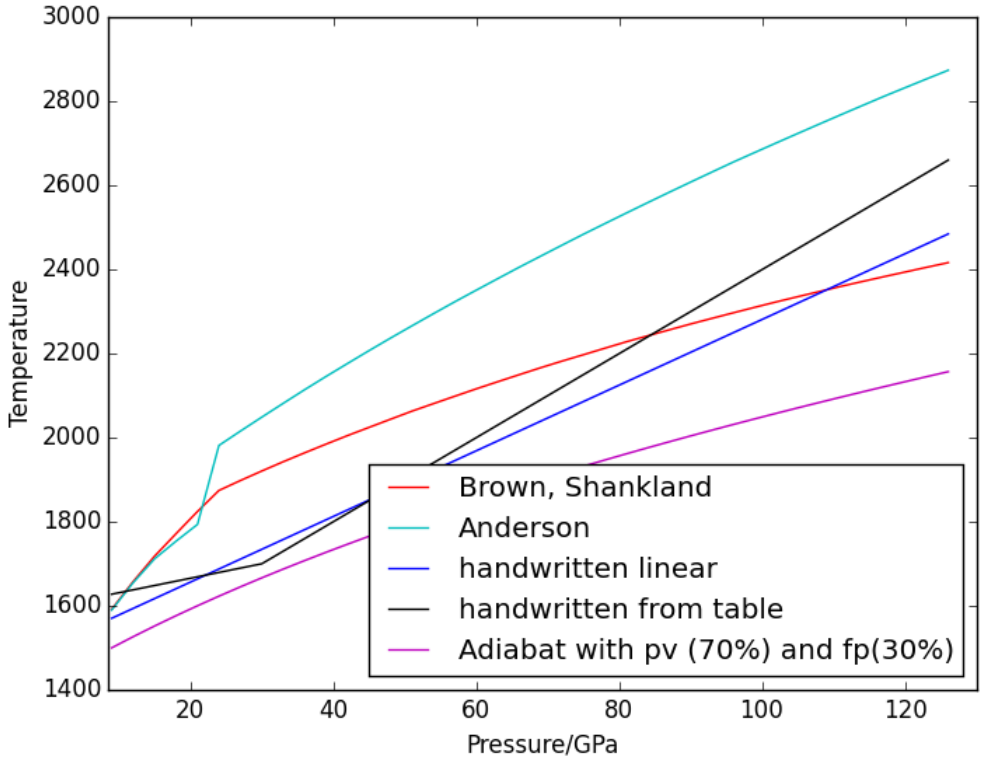
Inputs

Outputs

$$P, T, \chi \longrightarrow \mu, \gamma, G, H, F, S$$
$$\rho, \alpha, K_T, K_S, C_p, C_v$$

# Geotherms

T = f(r or P)




examples/example_geotherms.py

# Mineral libraries

Parameter libraries are (amongst others) included for mantle mineral from Stixrude and Lithgow-Bertelloni (2011) and Holland & Powell (2011, 2013).

Exact parameters depend on the equation of state.

Easy to add your own minerals.

Note: everything in BurnMan is in SI units.

```
class mg_perovskite (Mineral):
    def __init__(self):
        formula='MgSiO3'
        formula = dictionarize_formula(formula)
        self.params = {
            'name': 'Mg_Perovskite',
            'formula': formula,
            'equation_of_state': 'slb3',
            'F_0': -1368000.0 ,
            'V_0': 2.445e-05 ,
            'K_0': 2.51e+11 ,
            'Kprime_0': 4.1 ,
            'Debye_0': 905.0 ,
            'grueneisen_0': 1.57 ,
            'q_0': 1.1 ,
            'G_0': 1.73e+11 ,
            'Gprime_0': 1.7 ,
            'eta_s_0': 2.6 ,
            'n': sum(formula.values()),
            'molar_mass': formula_mass(formula, atomic_masses)}

        self.uncertainties = {
            'err_F_0': 1000.0 ,
            'err_V_0': 0.0 ,
            'err_K_0': 3000000000.0 ,
            'err_K_prime_0': 0.1 ,
            'err_Debye_0': 5.0 ,
            'err_grueneisen_0': 0.05 ,
            'err_q_0': 0.3 ,
            'err_G_0': 2000000000.0 ,
            'err_Gprime_0': 0.0 ,
            'err_eta_s_0': 0.3 }
        Mineral.__init__(self)
```

# Solid solutions

Different models to compute the state of a solid solution:

- Ideal solution
- (A)symmetric regular solution (Holland & Powell, 2003)
- Subregular solution (Helffrich and Wood, 1993)

```
class mg_fe_perovskite(SolidSolution):
    def __init__(self, molar_fractions=None):
        self.name='magnesium silicate perovskite/bridgmanite'
        self.type='symmetric'
        self.endmembers = [[mg_perovskite(), '[Mg][Si]O3'],[fe_perovskite(), '[Fe][Si]O3'],[al_perovskite(), '[Al][Al]O3']]
        self.enthalpy_interaction=[[0.0, 116.0e3],[0.0]]

        SolidSolution.__init__(self, molar_fractions)
```

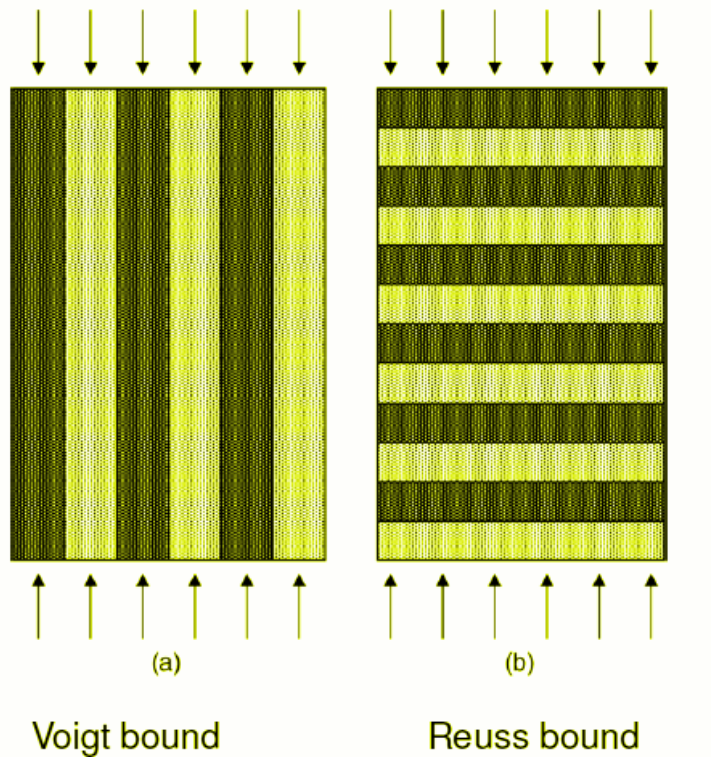
# Composites (or rocks)

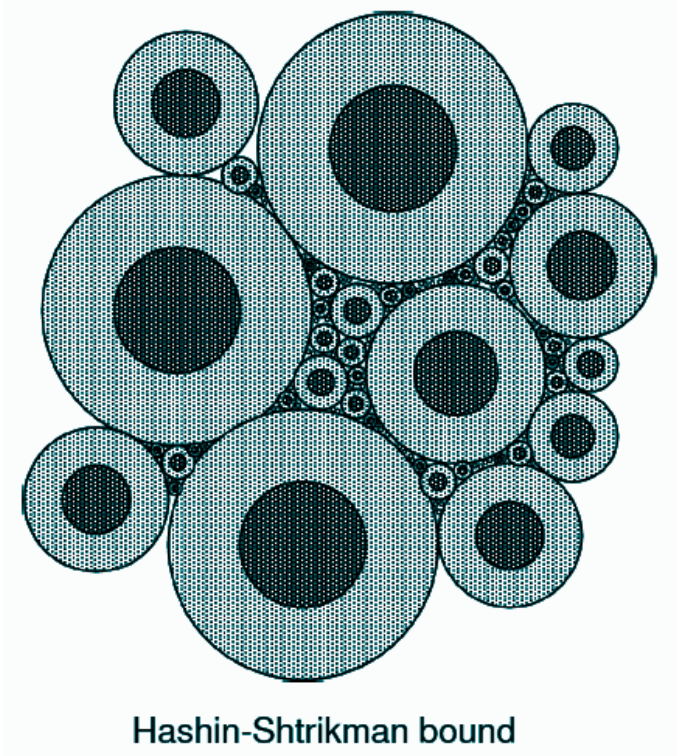
```
#Example: two simple fixed minerals
amount_perovskite = 0.95
rock = burnman.Composite([amount_perovskite, 1.0-amount_perovskite],
                         [minerals.SLB_2011.mg_perovskite(), minerals.SLB_2011.periclase()])


#Example: Mixing solid solutions
# Defining a rock using a predefined solid solution from the mineral library database.
preset_solidsolution=minerals.SLB_2011.mg_fe_perovskite()
# The line below is optional to see which endmembers (and in which order) are in the solid solution
preset_solidsolution.set_composition([0.9,0.1,0.]) # Set molar_fraction of mg_perovskite, fe_perovskite and al_perovskite
rock = burnman.Composite([0.8, 0.2], phases=[preset_solidsolution, minerals.SLB_2011.periclase()])
```

We have some combination of minerals/solid solutions (a rock) and would like to know its:

- density
- bulk modulus
- shear modulus
- seismic wavespeeds

# Averaging schemes

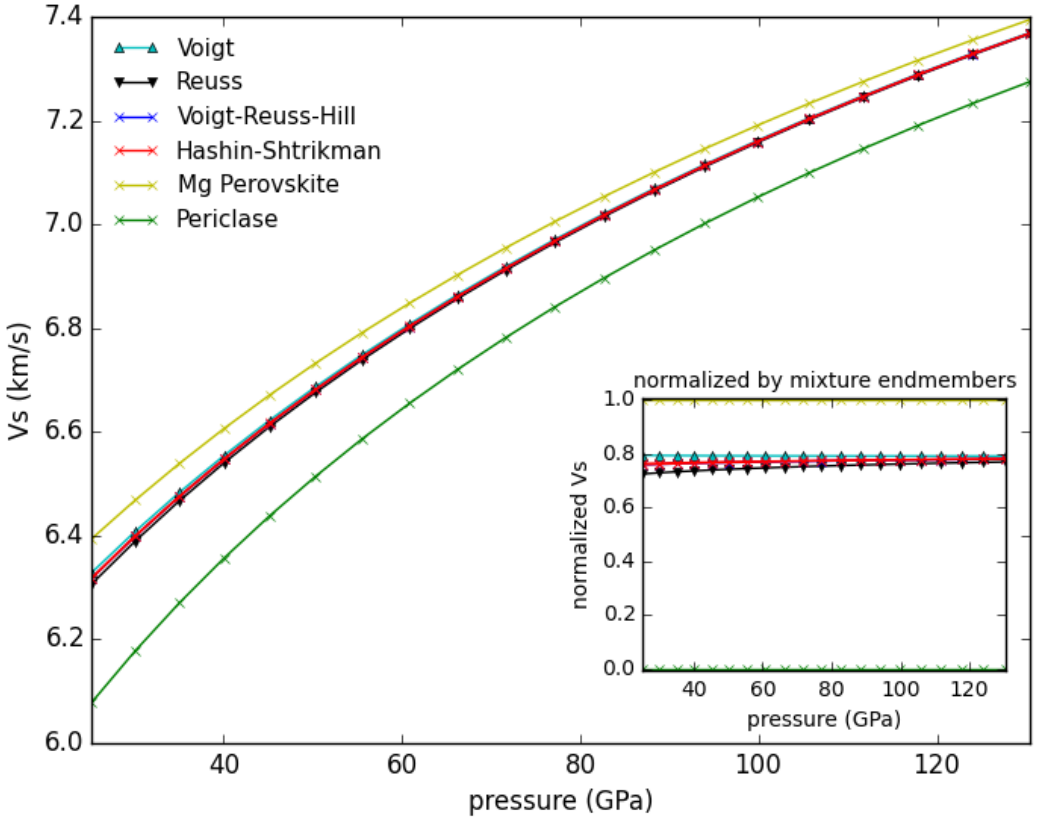



http://petrowiki.spe.org/

# Averaging schemes

- Example: different ways to mix a rock made out of 40% periclase and 60% Mg-perovskite
- Does the choice of averaging scheme matter? Sometimes!




examples/example_averaging.py

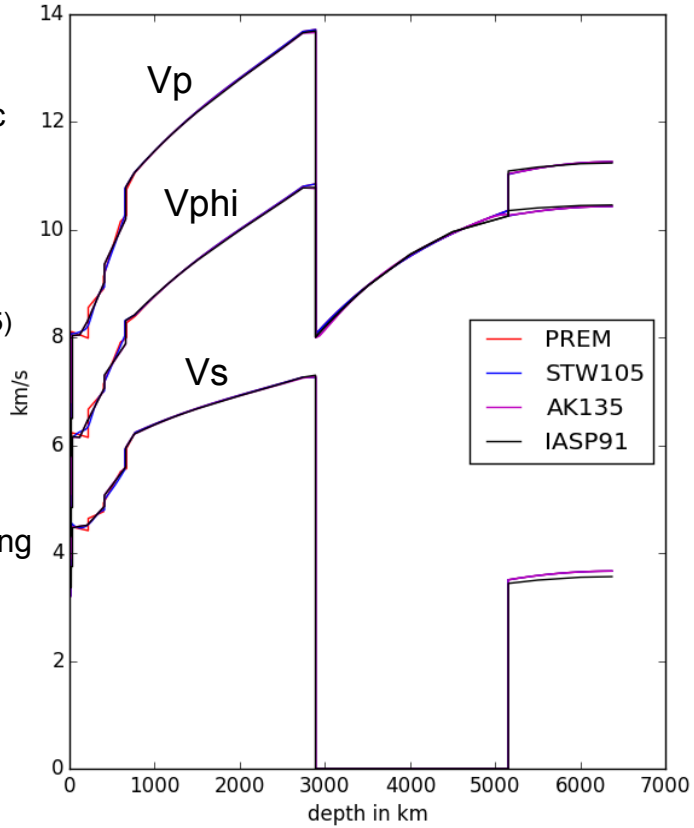
# Seismic models

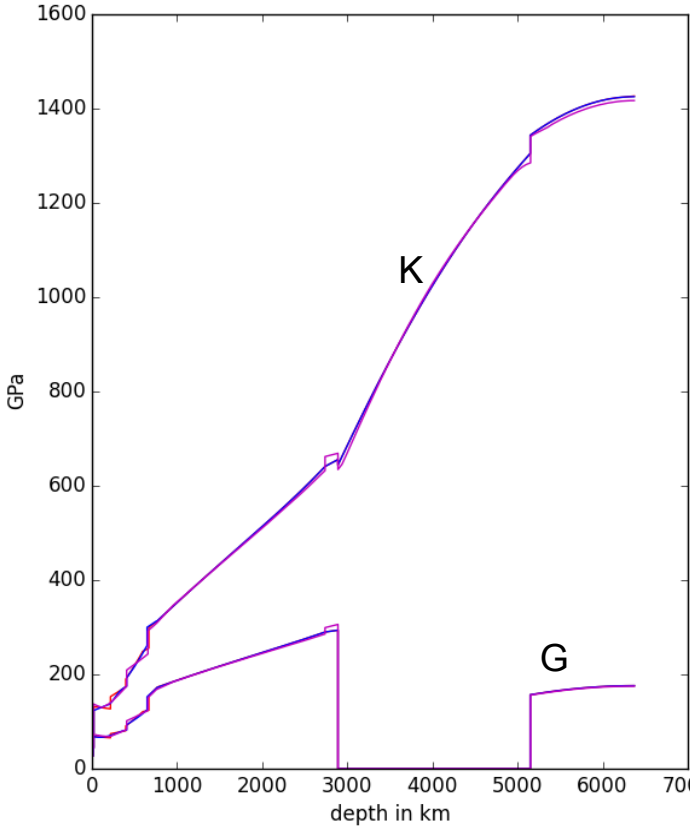
Currently 1D radial models only. Models can be queried for seismic moduli when density is included.

PREM Dziewonski & Anderson (1981)
STW105 Kustowski, Ekström and Dziewonski (2008)
AK135 Kennett, Engdahl & Buland (1995)
IASP91 Kennett & Engdahl (1991)

Note: models are in SI units in BurnMan, but here converted during plotting.

examples/example_seismic.py



# User defined modules

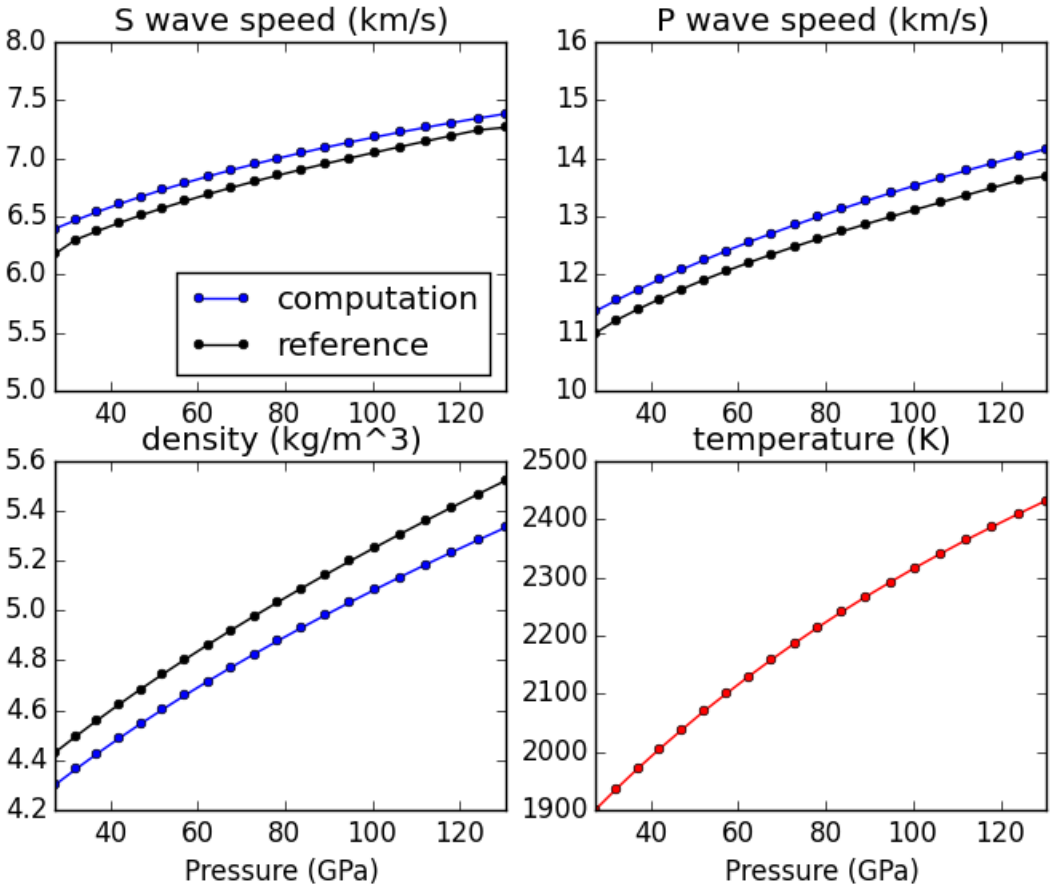
- equations of state
- mineral  and solid solution libraries
- solid solution models
- geotherms
- seismic models
- averaging schemes
- layers within planet

And contribute them to BurnMan for others to use!

# Part 2: Some more complete examples

# Example script

This example illustrates defining a composition and geotherm and computing seismic properties for the lowermost mantle and compare to PREM.




examples/example_beginner.py

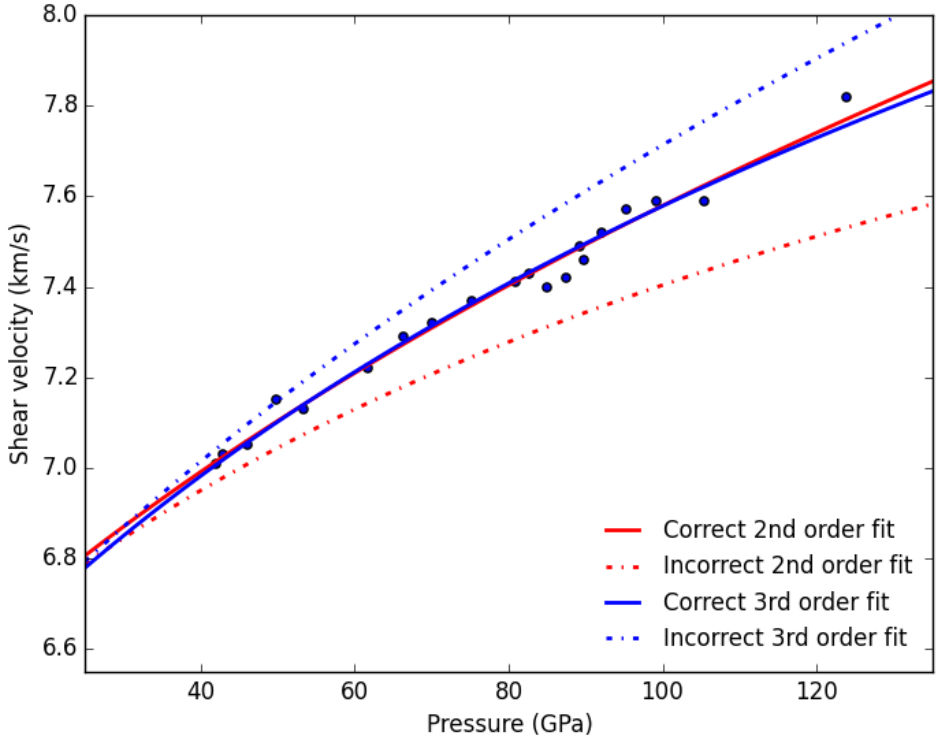
examples/example_beginner.py

```
import numpy as np
import matplotlib.pyplot as plt

import burnman
from burnman import minerals

# For the preset minerals from the SLB_2011, the equation of state formulation
# from Stixrude and Lithgow-Bertolloni (2005) will be used.
rock = burnman.Composite([0.8, 0.2], [minerals.SLB_2011.mg_perovskite(),
                                      minerals.SLB_2011.periclase()])

# Here we create and load the PREM seismic velocity model, which will be
# used for comparison with the seismic velocities of the "rock" composite
seismic_model = burnman.seismic.PREM()

# We create an array of 20 depths at which we want to evaluate PREM, and then
# query the seismic model for the pressure, density, P wave speed, S wave
# speed, and bulk sound velocity at those depths
depths = np.linspace(750e3, 2800e3, 20)
pressure, seis_rho, seis_vp, seis_vs, seis_vphi = seismic_model.evaluate_all_at(depths)

# Here we use the Brown & Shankland (1981) geotherm for mapping temperature to pressure
temperature = burnman.geotherm.brown_shankland(pressure)

# Here is the step which does the heavy lifting.
density, vp, vs, vphi, K, G = burnman.velocities_from_rock(rock, pressure, temperature)
```

# Reproducibility

One of the goals of BurnMan is to be able to reproduce studies, and use parameters published by previous studies in a self-consistent way.

This example illustrates the importance of using the same equation-of-state as was used when fitting the data. This is especially important when extrapolating to high pressures.



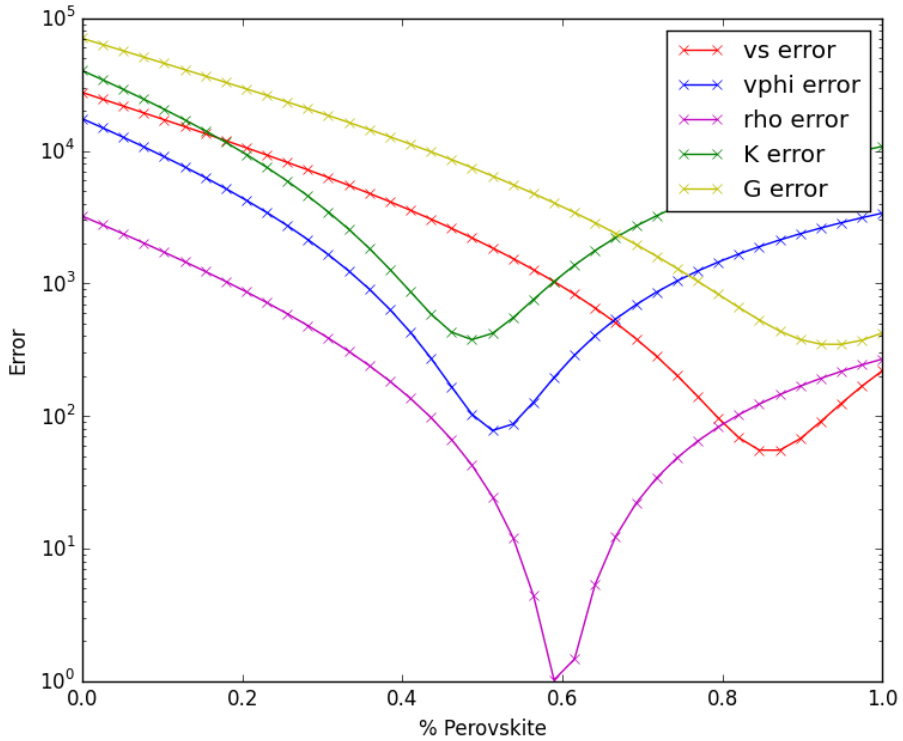

misc/paper_fit_data.py

# Mg/Si ratio in the lower mantle

examples/example_optimize_pv.py

Goal: Finding the ratio of bridgmanite (perovskite) to ferropericlase in the lower mantle by fitting PREM.

Using mineral parameters from Stixrude & Lithgow-Bertelloni (2011).



examples/example_optimize_pv.py

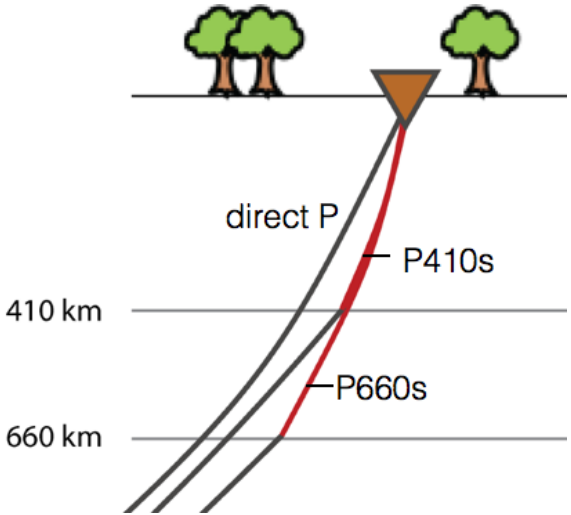
```
import numpy as np
import matplotlib.pyplot as plt

import burnman
from burnman import minerals


# Define reference model and depth to evaluate
seismic_model = burnman.seismic.PREM()
number_of_points = 20
depths = np.linspace(700e3,2800e3, number_of_points)
seis_p, seis_rho, seis_vp, seis_vs, seis_vphi, seis_K, seis_G = \
        seismic_model.evaluate(['pressure','density','v_p','v_s','v_phi','K','G'],depths)

#Define geotherm
temperature = burnman.geotherm.brown_shankland(seis_p)

#Define solid solutions
perovskite=minerals.SLB_2011.mg_fe_perovskite()
perovskite.set_composition([0.94,0.06,0.]) # Set molar_fraction of mg_perovskite, fe_perovskite and al_perovskite
ferropericlase=minerals.SLB_2011.ferropericlase()
ferropericlase.set_composition([0.8,0.2]) # Set molar_fraction of MgO and FeO

def material_error(amount_perovskite):
    #Define composite using the values
    rock = burnman.Composite([amount_perovskite, 1.0-amount_perovskite],
                             [perovskite, ferropericlase])

    # Compute velocities
    mat_rho, mat_vp, mat_vs, mat_vphi, mat_K, mat_G = \
        burnman.velocities_from_rock(rock, seis_p, temperature, burnman.averaging_schemes.VoigtReussHill())

    print "Calculations are done for:"
    rock.debug_print()

    # Calculate errors
    [vs_err, vphi_err, rho_err, K_err, G_err] = \
        burnman.compare_l2(depths, [mat_vs,mat_vphi,mat_rho, mat_K, mat_G], [seis_vs,seis_vphi,seis_rho, seis_K, seis_G])

    return vs_err, vphi_err, rho_err, K_err, G_err

# Run through fractions of perovskite
xx=np.linspace(0.0, 1.0, 40)
errs=np.array([material_error(x) for x in xx])
```

# Part 3: Research Projects

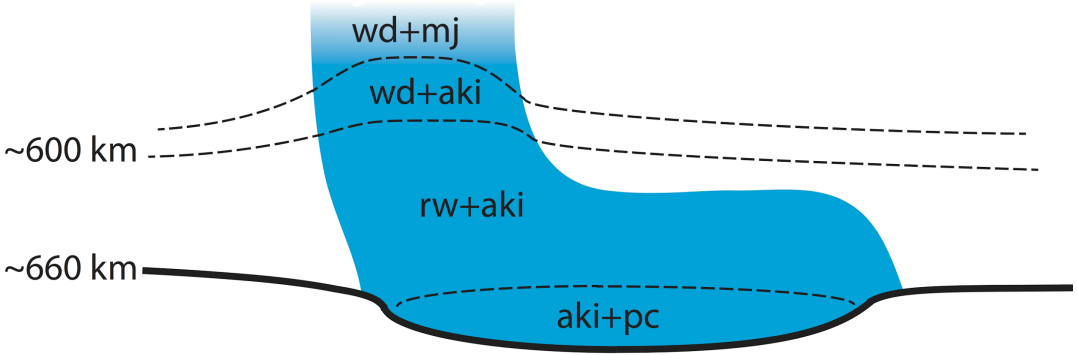
# Application to Research:
# Predicting velocity and density contrasts at 660 km

Sanne

P-to-s conversions or receiver functions

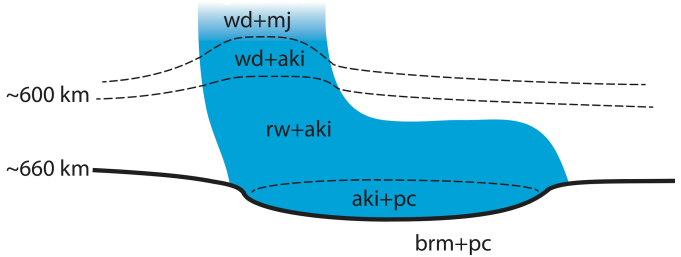



Akimotoite at the bottom of a cold slab

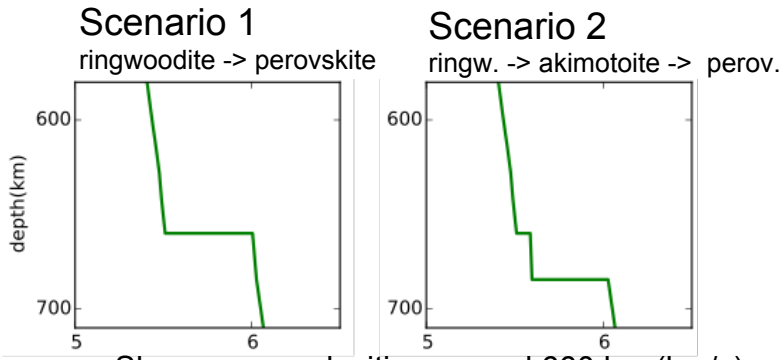


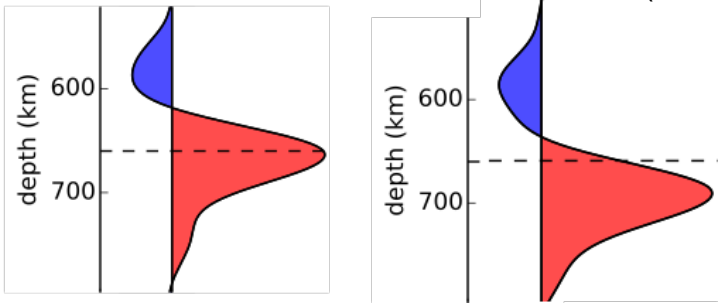

wd = wadselyite
mj = majorite
aki = akimotoite
rw = ringwoodite
pc = periclase
brm = bridgmanite or perovskite

# Application to Research:
# Predicting velocity and density contrasts at 660 km

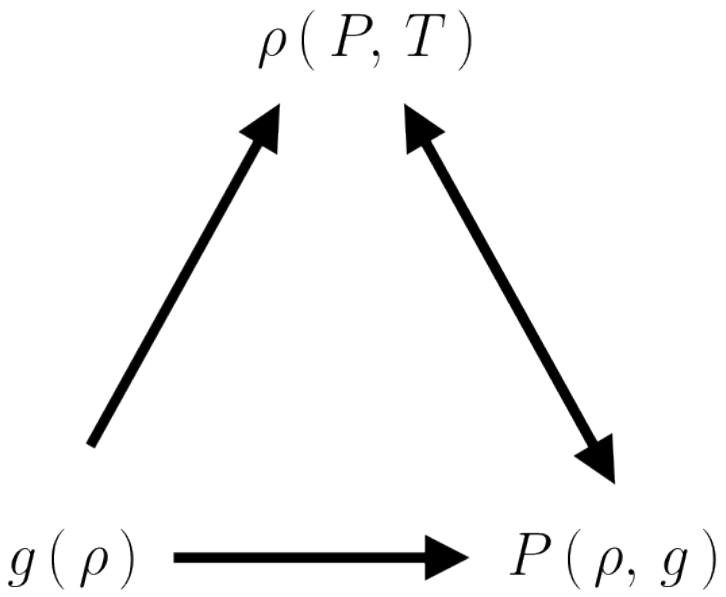


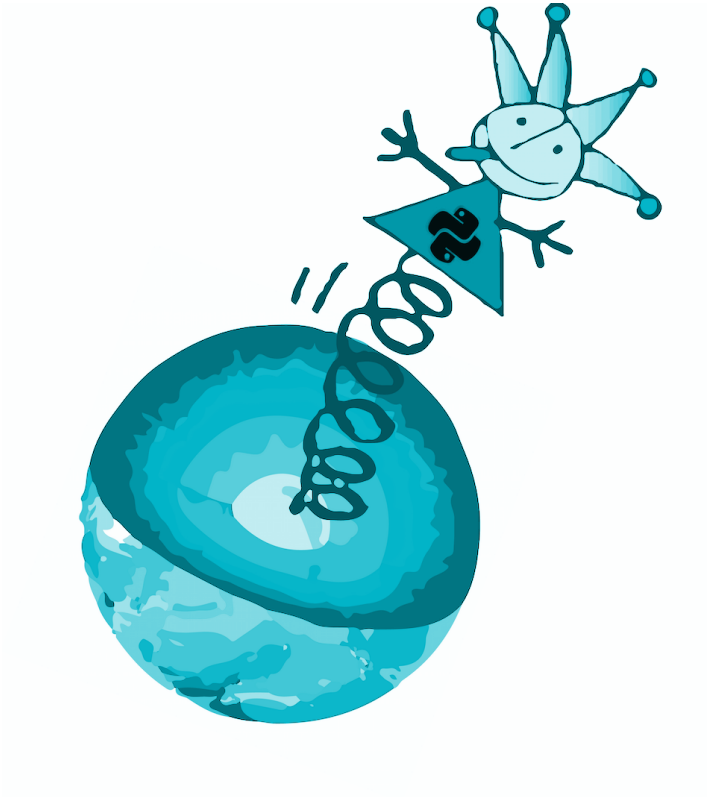

```
#Example computing impedance constrasts at 660 km

# Defining a rock using a predefined solid solution from the mineral library database.
pv=minerals.SLB_2011.mg_fe_perovskite(molar_fractions=[0.9,0.1,0.])
aki=minerals.SLB_2011.akimotoite(molar_fractions=[0.9,0.1,0.])
ring=minerals.SLB_2011.mg_fe_ringwoodite(molar_fractions=[0.9,0.1])
pc=minerals.SLB_2011.ferropericlase(molar_fractions=[0.9,0.1])

#Define Composites
rock = burnman.Composite([0.8, 0.2], phases=[pv, pc])
rock2 = burnman.Composite([0.8, 0.2], phases=[aki, pc])
rock3 = burnman.Composite([0.6, 0.4], phases=[ring,aki])
#seismic model for comparison:
# pick from .prem() .slow() .fast() (see burnman/seismic.py)

number_of_points = 20 #set on how many depth slices the computations should be done
# we will do our computation and comparison at the following depth values:
depths = np.linspace(500e3, 800e3, number_of_points)
```



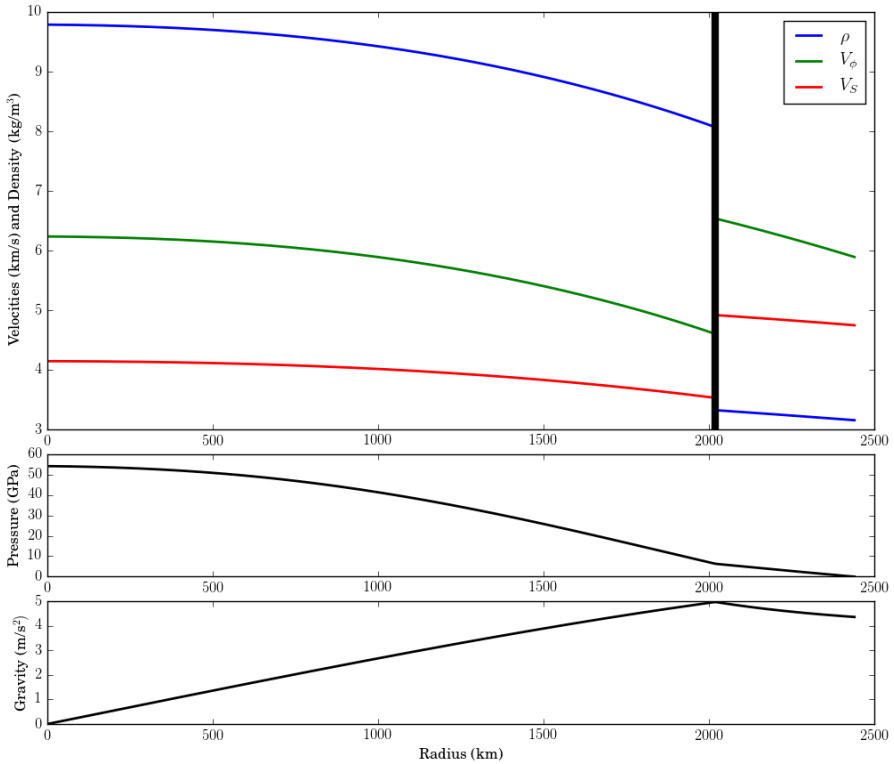
# Planetary reference models



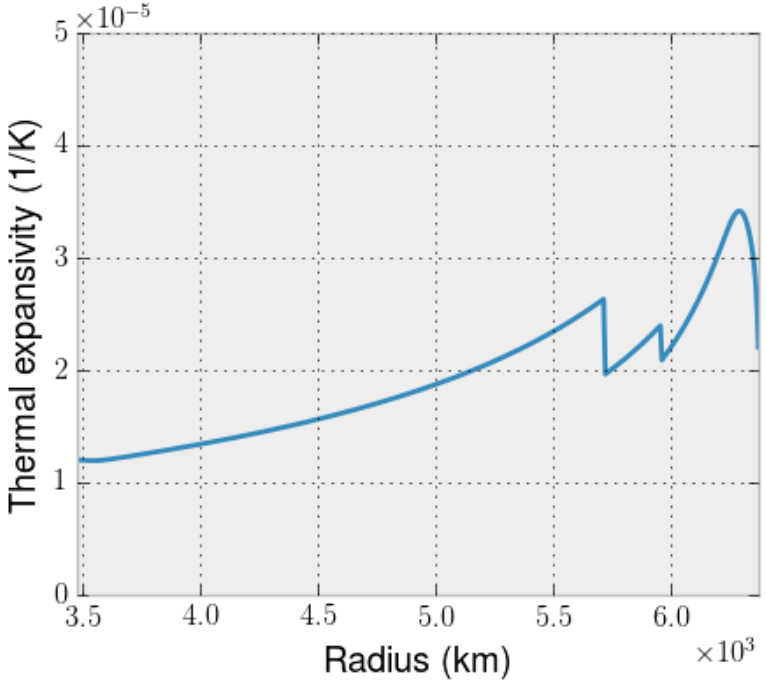



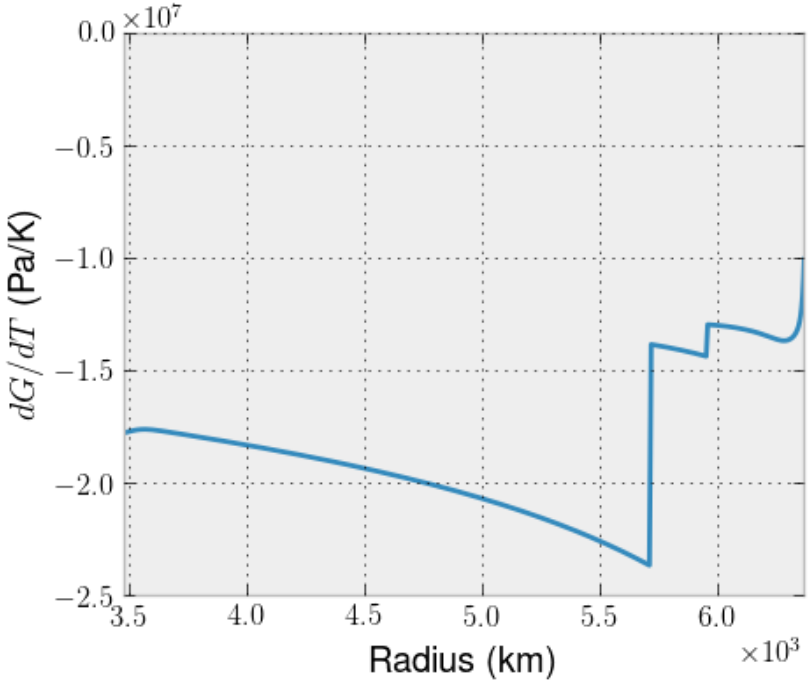
# Example: internal structure of Mercury

rock=?



# Reference model for mantle convection simulation



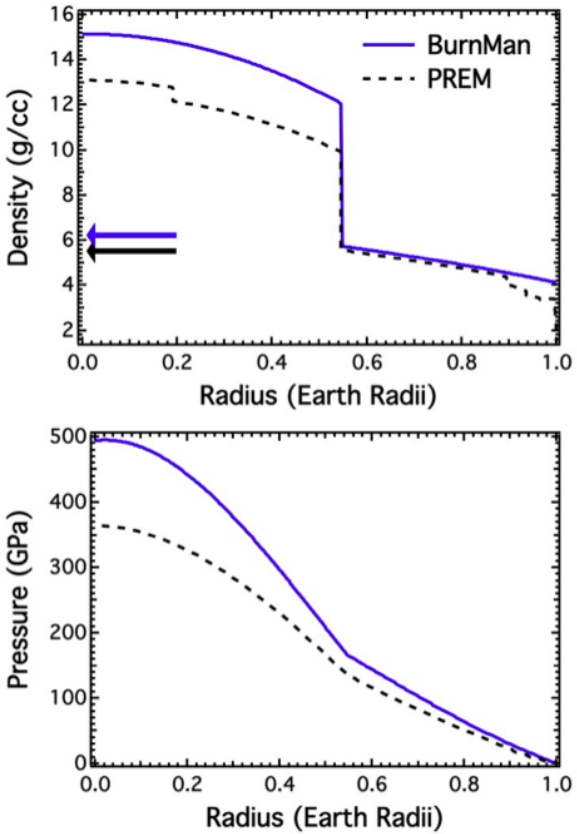
Cayman

# Application to Research: How Interior Composition Affects Exoplanet Observables

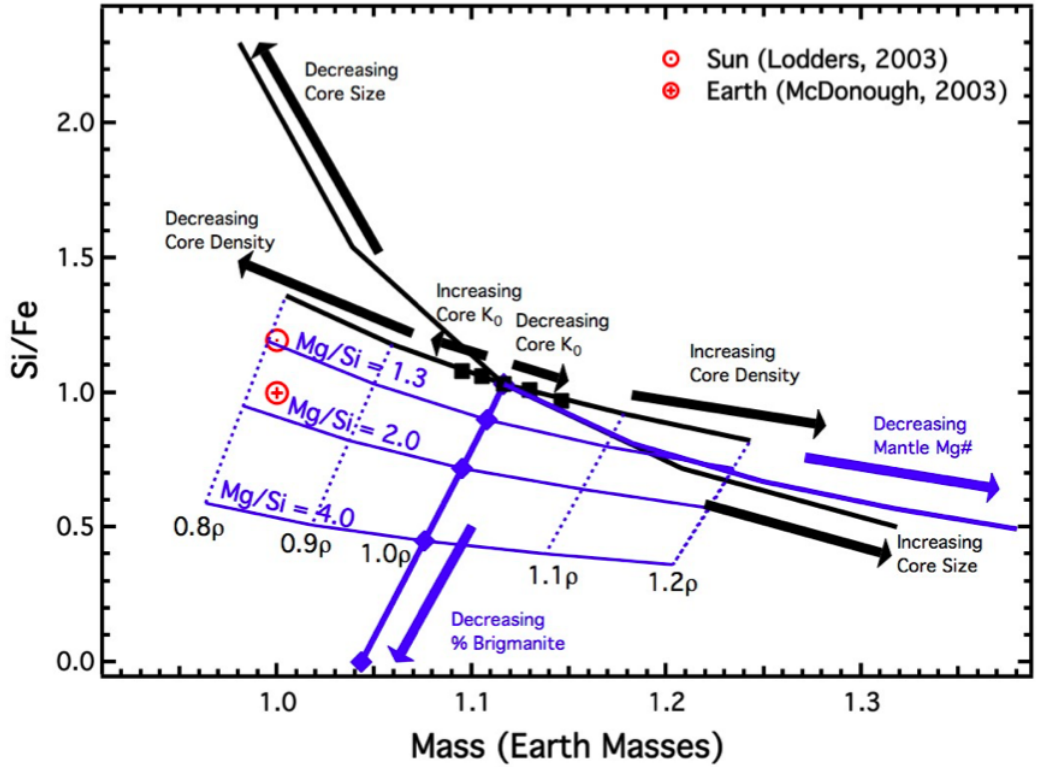
$$\frac{dm(r)}{dr} = 4\pi r^2 \rho(r)$$

$$\frac{dP(r)}{dr} = \frac{-Gm(r)\rho(r)}{r^2}$$

$$P(r) = f(\rho(r), T(r))$$



# Application to Research: How Interior Composition Affects Exoplanet Observables



# The Future

- release at the end of the year:
  - Clean up the hierarchy of different materials for clarity and consistency
  - Performance improvements
  - Python 3 compatibility
- long term:
  - Gibbs free energy minimization and phase equilibria
  - coupling with ASPECT
  - 3D seismic variations

# Thank you!

This collaboration is initiated at and funded through CIDER (www.deep-earth.org).

BurnMan is hosted by Computational Infrastructure for Geodynamics (CIG).

CIDER
Cooperative Institute for Dynamic Earth Research

Thanks to many for discussions and input!

Anyone is welcome to get involved! If you have an idea, contact us!

CIG

Cottaar, S., Heister, T., Rose, I., and Unterborn, C:
*BurnMan - a lower mantle mineral physics toolkit*
Geochemistry, Geophysics, Geosystems 15.4 (2014): 1164-1179.

# Section 4: Live Tutorial

- tutorial demonstration
- you can find them in burnman under tutorial/step_*.py