strcutCalc
a program to generate a priori structure models of Mars

A. Rivoldini, P. Lognonné, Antoine Mocquet, and the MSS team

Motivation

- need for a large set (>>1000) of plausible interior structure models for blind tests

- could be provided by science team members following (often changing) requirements from MSS

- or generated on the fly by MSS

Prior models of Mars

- should agree with average density
- compatible with thought mantle composition of Mars
- and thermal state
- have liquid layer in core made of Fe-S

MSS requirements

- user provided crust structure model
- user provided elastic properties for mantle along given reference mantle temperature as a function of p (from Perple_X, MMA-EoS, .. for a given composition)
- user provided temperature deviation from reference temperature profile for upper mantle

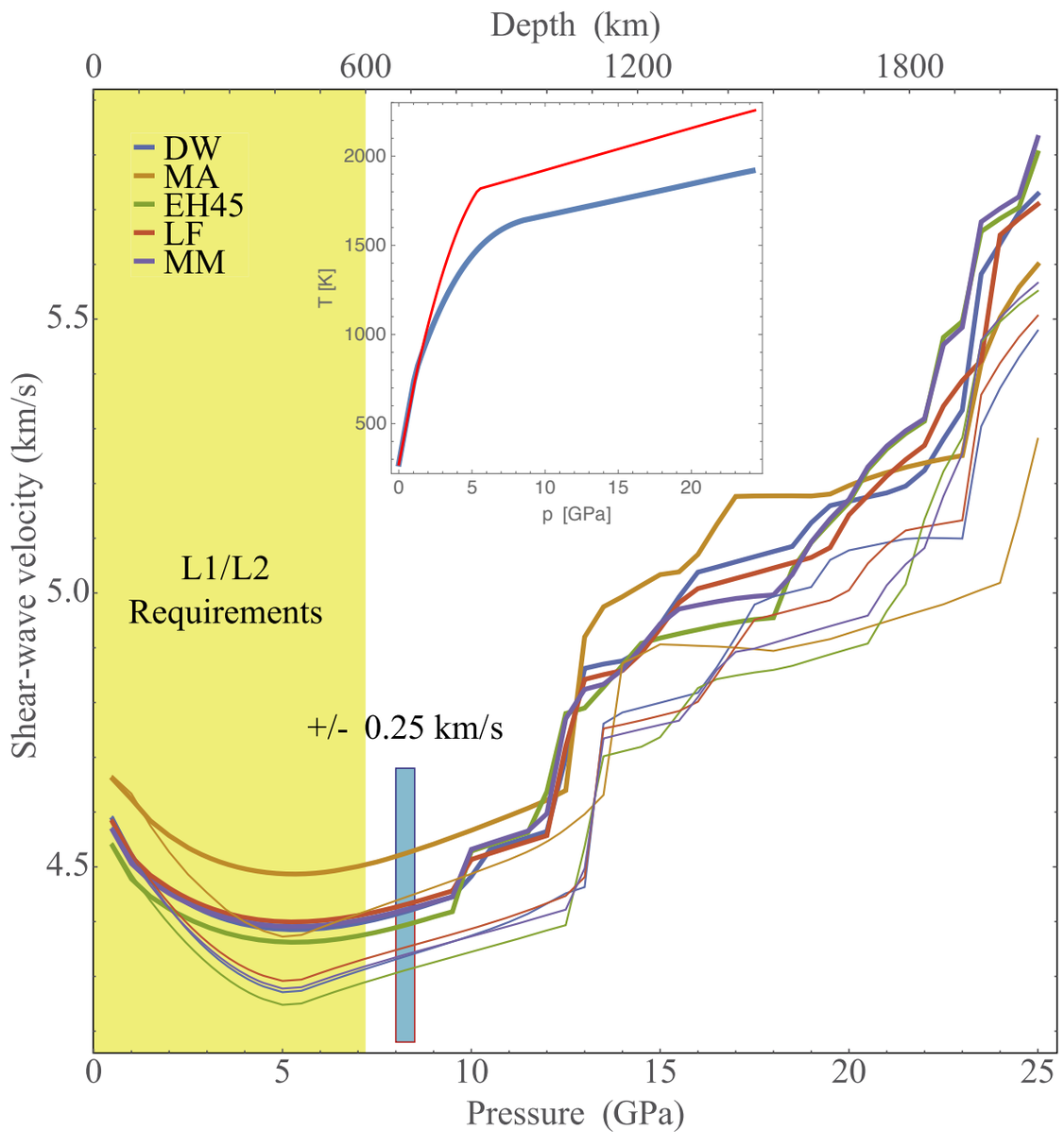
→By combining the above 3 inputs with chosen core radii a large number of models can be constructed

Upper mantle velocities

- predicted seismic velocity variations at depth shallower than 600km are smaller than precision expected from SEIS

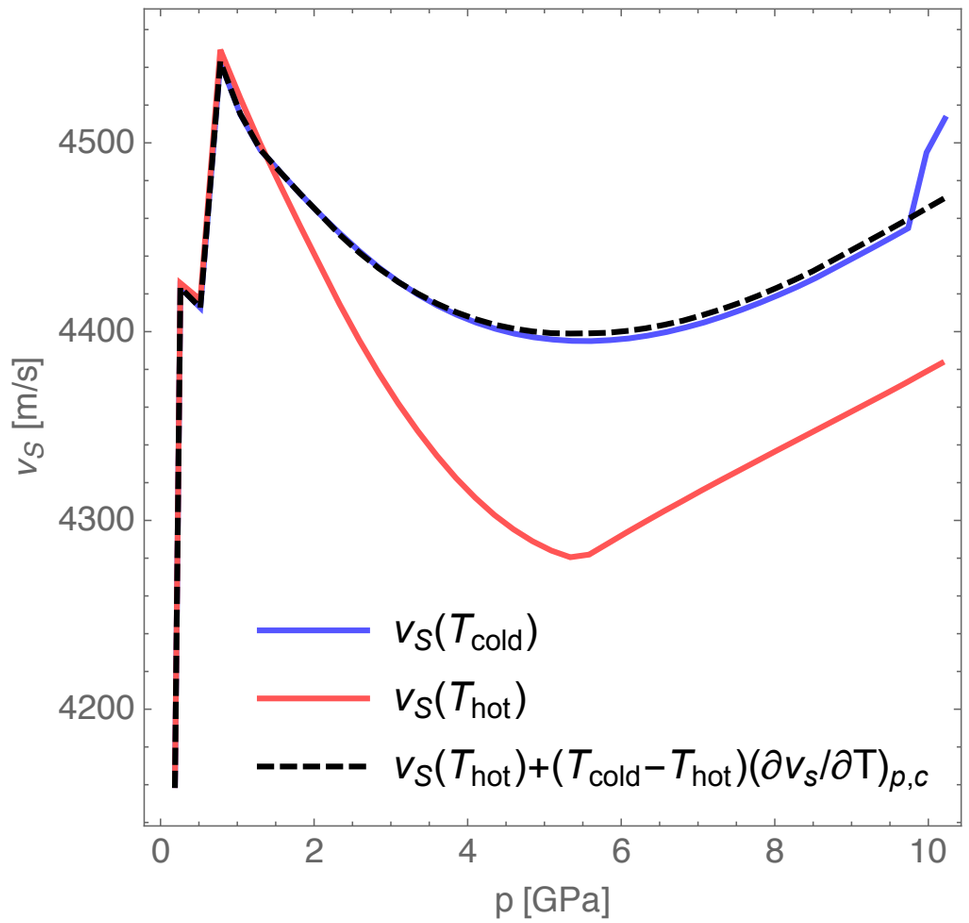
- profiles are smooth and are not significantly affected by upper mantle phase transitions

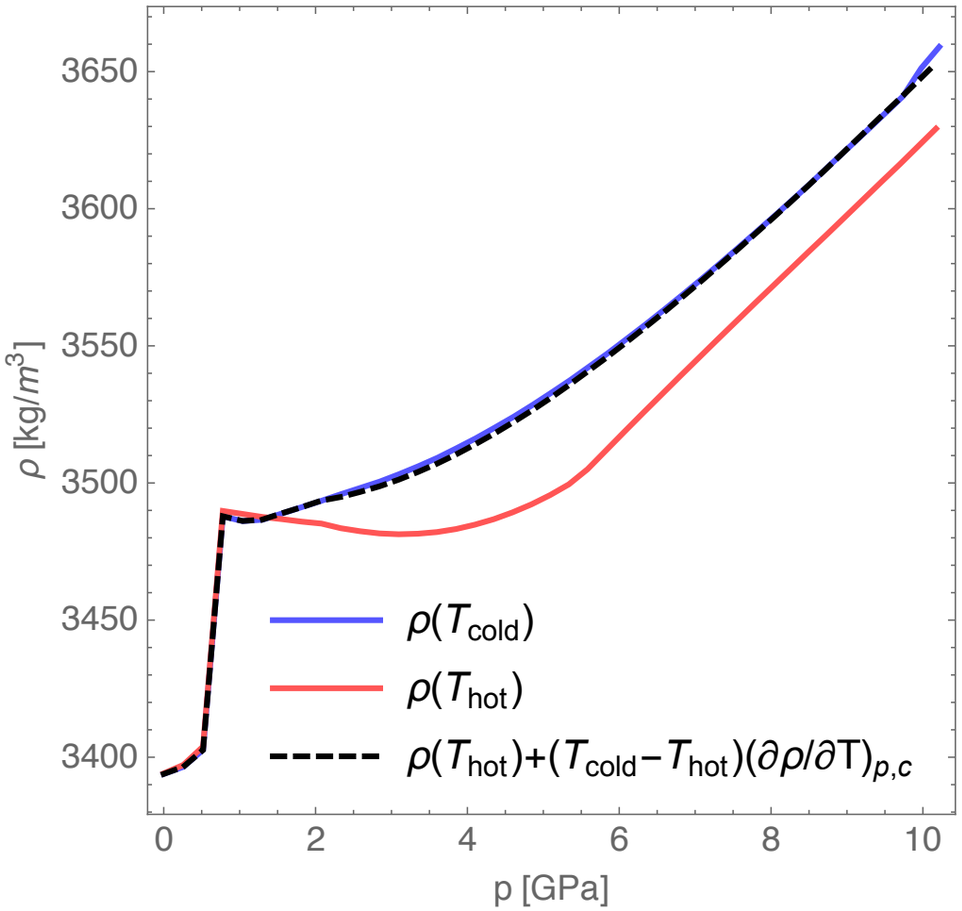
- effect of temperature is much larger than effect of composition



Effect of T on $v_{p/s}$ and ρ is almost linear

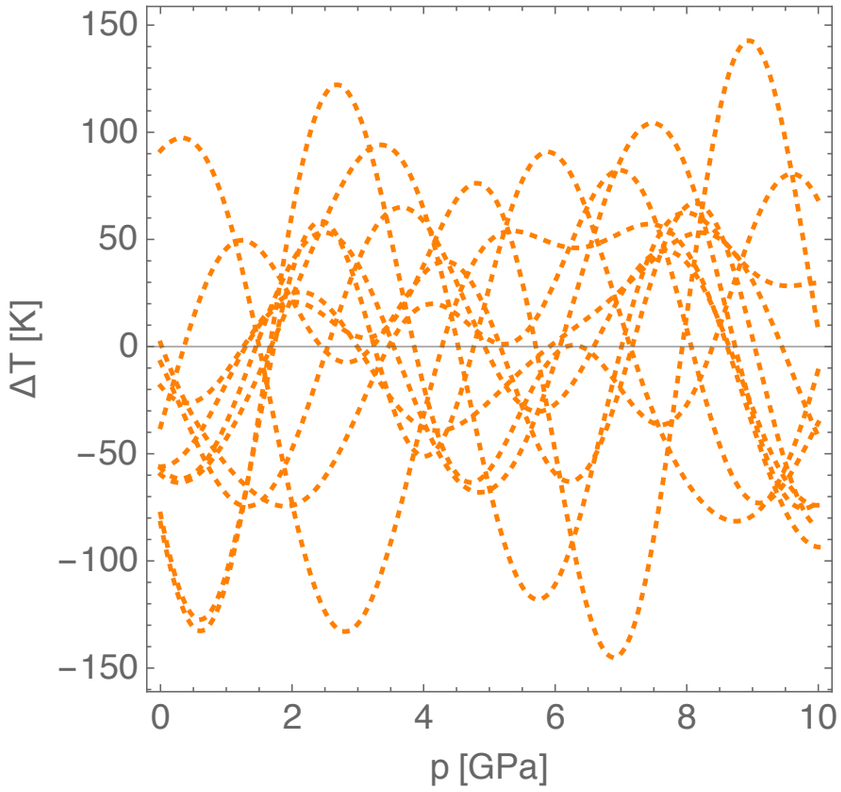
$$v_s(p, T + \Delta T) = v_s(p, T) + \left.\frac{\partial v_s(p, T)}{\partial T}\right|_{p,c} \Delta T + \ldots$$

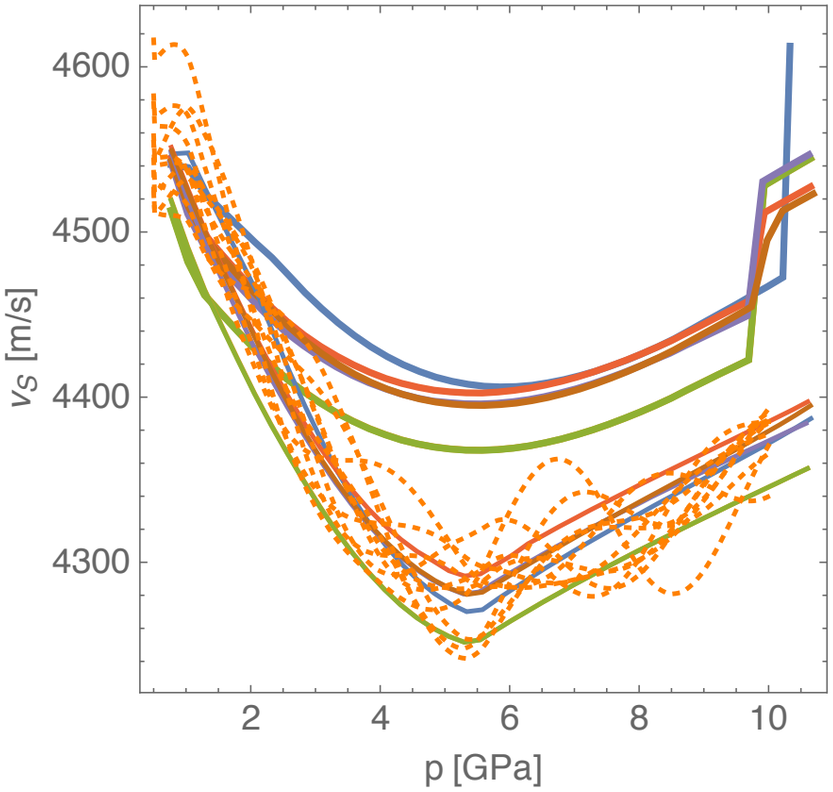




Generate upper mantle models by providing temperature deviation profiles

- from pre-calculated profiles of density, seismic velocities, and iso-chemical partial derivatives with respect to temperature along end-member temperature profiles for a given set of mantle compositions





strcutCalc

- computes pressure, temperature, density, seismic velocities profiles for the whole planet and planet moment of inertia and core light element weight fraction

- requires user provided files for crust structure, upper mantle temperature deviation profile, mantle mineralogy, and core radius

- core model assumes liquid convecting Fe-S

Implementation

- Fortran 2003 (compiles with gfortran 8.1)
- solves Poisson’s and hydrostatic pressure equation in the whole planet and solves adiabatic temperature equation in the core
- ode’s with boundary conditions are solved with BVP_SOLVER (Fortran 90/95, Shampine et al 2006)

crust structure file:

- contains density[kg/m^3], v_p[m/s], and v_s[m/s] as a function of depth [km]

- from surface down to depth of crust thickness

```
$ more crustModels/crust.dat
d [km]  rho[kg/m]       vp[m/s]         vs[m/s]
 0.00   2600.00         5400.00         3117.69
10.00   2600.00         5470.00         3158.11
20.00   2600.00         5540.00         3198.52
30.00   2900.00         6750.00         3897.11
40.00   2900.00         6800.00         3925.98
50.00   2900.00         6850.00         3954.85
```

lithosphere temperature file:

- contains temperature deviation as a function of depth
- from bottom of crust on to a depth of less than about 800km (p<~8GPa)

```
$ more lithosphereModels/lithosphere.dat
d[km]   deltaT [K]
50.      0.
100.    10.4
150.    20.34
200.    29.39
250.    37.16
300.    43.3
350.    47.55
400.    49.73
450.    49.73
500.    47.55
550.    43.3
600.    37.16
650.    29.39
700.    20.34
750.    10.4
800.    0.
```

mantle mineralogy file:

- contains p,T, ρ, v_p, v_s, and their partial derivatives with respect to temperature as function of pressure (p<~25GPa)

```
$ more mantleCompositions/TAY_Thot.dat
p [GPa] T[K]       rho[kg/m3] vp[m/s]   vs[m/s]     drhodT[kg/m3/K] dvpdT[m/s/K] dsvdT[m/s/K]
0.00    272.15     3394.10    7064.40   3464.30      -0.06           -0.30        -0.16
0.25    383.17     3397.20    7745.90   4425.70      -0.08           -0.42        -0.27
0.51    494.19     3403.90    7739.30   4416.90      -0.08           -0.46        -0.30
0.77    605.21     3489.80    7942.40   4549.30      -0.09           -0.51        -0.32
1.04    716.23     3488.70    7919.30   4523.60      -0.10           -0.53        -0.33
1.30    816.52     3487.60    7896.80   4499.40      -0.10           -0.54        -0.33
1.56    906.88     3486.80    7877.10   4477.40      -0.10           -0.54        -0.34
1.81    993.39     3485.90    7857.30   4455.90      -0.10           -0.55        -0.34
2.07    1076.05    3485.20    7838.40   4435.10      -0.10           -0.56        -0.35
2.33    1154.85    3483.50    7818.40   4414.50      -0.10           -0.56        -0.35
2.58    1229.79    3482.40    7800.80   4395.50      -0.11           -0.56        -0.35
2.84    1300.87    3481.60    7785.90   4378.00      -0.11           -0.57        -0.35
3.09    1368.10    3481.30    7774.10   4362.00      -0.11           -0.57        -0.35
3.34    1431.47    3481.50    7764.60   4347.50      -0.11           -0.57        -0.36
3.59    1490.99    3482.10    7757.10   4334.30      -0.11           -0.57        -0.36
3.84    1546.65    3483.20    7751.90   4322.40      -0.11           -0.57        -0.36
4.09    1598.45    3484.80    7749.00   4312.00      -0.11           -0.57        -0.36
4.34    1646.39    3486.80    7748.20   4302.90      -0.11           -0.57        -0.36
4.59    1690.48    3489.30    7749.70   4295.30      -0.11           -0.57        -0.36
4.84    1730.72    3492.20    7753.30   4289.00      -0.11           -0.57        -0.36
5.09    1767.09    3495.60    7759.00   4284.00      -0.11           -0.57        -0.36
5.33    1799.61    3499.50    7766.90   4280.50      -0.11           -0.56        -0.36
5.58    1818.36    3505.00    7782.40   4281.90      -0.11           -0.56        -0.36
5.82    1823.98    3511.90    7805.10   4287.80      -0.10           -0.55        -0.36
6.07    1829.60    3518.80    7827.30   4293.70      -0.10           -0.55        -0.36
6.31    1835.21    3525.60    7849.00   4299.40      -0.10           -0.54        -0.35
6.56    1840.83    3532.30    7870.40   4305.00      -0.10           -0.54        -0.35
```

usage:

```
$./strcutCalc usage
 usage: coreRadius([1300.e3,2100.e3]m) fileNameCrustModel fileNameLithosphereModel fileNameMantleMineralogy
[fileNameResult]

$ ./strcutCalc 1800.e3 crustModels/crust.dat lithosphereModels/lithosphere.dat mantleCompositions/TAY_Thot.dat
xS=18.045 MOI=0.3664 MOITEST=F error:0
    r[km]            g[m/s**2]      p[GPa]       T[K]          rho[kg/m**3]   vp[m/s]         vs[m/s]
    3389.500000      3.727866       0.000000     272.156100    2600.000000    5400.000000     3117.690000
    3377.000000      3.728156       0.121160     324.174317    2600.000000    5487.500000     3168.212500
    3364.500000      3.728551       0.242331     376.156056    2750.000000    6145.000000     3547.815000
    3352.000000      3.729052       0.363517     428.090062    2900.000000    6787.500000     3918.762500
    3339.500000      3.729661       0.484721     479.886035    2900.000000    6850.000000     3954.850000
    3339.500000      3.729661       0.484721     479.886035    3397.448951    7734.180463     4420.295474
    3152.000000      3.606373       2.876820    1345.448821    3477.619546    7763.960129     4363.114553
    2964.500000      3.494262       5.193466    1831.404145    3491.565383    7733.425025     4264.041315
    2777.000000      3.390212       7.465703    1896.968701    3553.302078    7928.836912     4312.564866
    2589.500000      3.293508       9.711436    1914.206485    3616.616894    8130.666452     4372.948143
    2589.500000      3.293508       9.711436    1914.206485    3616.616894    8130.666452     4372.948143
    2392.125000      3.204100      12.051156    1969.672993    3688.258290    8344.593772     4439.197888
    2194.750000      3.123606      14.410450    2025.332284    3873.519155    8992.771928     4802.417836
    1997.375000      3.059398      16.790520    2081.322565    3944.821036    9219.700280     4891.276924
    1800.000000      3.030448      19.189908    2137.822682    4031.637983    9516.050414     5039.386124
    1800.000000      3.030448      19.189908    2137.822682    5778.080940    4943.914493        0.000000
    1350.000000      2.333467      26.338113    2286.449399    6044.656638    5219.104415        0.000000
     900.000000      1.584731      31.761712    2356.308666    6236.478479    5410.895300        0.000000
     450.000000      0.801181      35.147064    2380.133201    6352.825455    5524.237429        0.000000
       0.000000      0.000000      36.297928    2383.382681    6392.169772    5561.861085        0.000000
```

Available when?

- soon for MSS (beginning October)

- rest of science team as soon as MSS has finished testing