Operation of Fortran code for determining the elastic moduli from the resonances of a rectangular parallelepiped resonator, cylinder, or sphere.

The codes were compiled using microsoft visual studio .net combined with the Intel Fortran 9.0 compiler. The input file has the same name for all three codes, rusin.dat and must be in the same directory as the executable. Two output files will be produced after at least one iteration. They are rusout.dat, and rusio.dat. rusio.dat is a copy of the input file but with the fitted moduli (and dimensions) replacing the initial guesses, and the fitted frequencies replacing the column of zeros. It may be renamed rusin.dat using the ___io.bat file, and then a run can be started where the previous pass finished. Hitting any key stops iteration, and generates an orderly exit with the interim outputs in rusio.dat and rusout.dat. rusout.dat contains the results.

a) Input file:

Use this file to test the code. In order:

2=number of moduli (9 max).

0=number of dimension to be fit (0 or 3). Only the RPR code fits dimensions, so it should be set to 0 for the cylinder and sphere input files.

12 is the order of the basis set (16 max).

0 indicates a fit, any integer n up to 600 indicates compute n modes but do not fit.

1.3396 is the mass in grams.

1.00 is a convergence parameter-any positive real number works, the higher it is, the slower and more stable the convergence.

1 indicates output to screen (0 suppresses it).

the next nine 0's indicate that all moduli are free to float. Setting a 0 to 1 will lock that modulus to the initial guess–all moduli in this line are the orthorhombic equivalent. This is not implemented in the sphere code.

0.5 and 0.16 are the guesses for c11 and c44 in 10^{12} dynes/cm^2–for more moduli, one pass of the code will indicate which moduli are free in rusout.dat.

0.474481, 0.377003, 0.484186 are the dimension in cm

The remainder are frequencies in MHz–400 frequencies is the maximum, 0.is not used but must be a real number, and 1.00 indicates a weight of 1.00 for this mode–any real positive number is ok.

0. 0. 0. Indicates a mode that is missing but beleived to be present.

The input file follows. It is important to read the initial comment section of the code for essential information.

```
     Test
 2 0 12  0  1.339600 1.00 1 0 0 0 0 0 0 0 0 0
 0.5 0.16
  0.474481  0.377003  0.484186
  0.089937 0. 1.00
  0.122485 0. 0.00
  0.123037 0. 1.00
  0.133300 0. 1.00
  0.136562 0. 1.00
  0.140502 0. 1.00
  0.144324 0. 1.00
 0. 0. 0.
  0.150841 0. 1.00
  0.150964 0. 1.00
```

```
 0.162553 0. 1.00
 0.163018 0. 1.00
 0.164211 0. 1.00
 0.171321 0. 1.00
 0.190858 0. 1.00
 0.191871 0. 1.00
 0.194339 0. 1.00
 0.197951 0. 1.00
 0.198913 0. 1.00
 0.200511 0. 1.00
 0.203233 0. 1.00
 0.207026 0. 1.00
 0.207831 0. 1.00
 0.209198 0. 1.00
  0.209741 0. 1.00
```

b) Output file

In an abridged version of our output file (below) for an isotropic solid with two free moduli, note that the free moduli are indicated, but nine moduli are printed. `fex` are measured frequencies in MHz, `fr` are computed as fitted parameters by the code. These nine are the redundant "orthorhombic" set–that is, in this case, only `c11` and `c44` are independent–that produces the same elastic tensor as the free moduli. The code can also adjust dimensions with the constraint that the volume is fixed. This is a less stable mode of operation.

For a useful fit, five things must be true.

1)The fit must be predictive–if a mode is missing, and the code predicts it is there, one should be able to find it by re-measuring, or remounting the sample.

2) The `RMS error` should be below 0.8%, often below 0.2%–sometimes as low as 0.03%.

3)"`chisquare increased 2% by the...`" must be small–the largest number in the first column below "`chisquare...`" is computed from the effective curvature of the minimum in elastic-modulus space for `c11`, the next column for the next free modulus (in this case `c44`) etc. The largest number in each column represents a real-world measure of the accuracy of the measurement tested by much experience–the accuracy is very definitely *not* the rms error.

4) There must be many modes that are not pure shear. Note that the first mode is pure shear (`df/dmoduli` is 0. for `c11` and 1.00 for `c44`–again, these derivatives are in order of the free moduli, just as are the chisquare columns). But the 7^{th} mode is 41% `c11`, so it provides a strong constraint for `c11`. Typically, one must use 40 modes for orthorhombic symmetry, but maybe only 15 for isotropic.

5) The *Q* of the modes must be high–of order a few hundred and up–we have observed a *Q* of 1.5×10^6 for diamond.

```
TEST
free moduli are c11, c44
using 11 order polynomials   mass= 1.3396 gm rho=15.467 gm/cc

 n    fex     fr   %err wt k i   df/d(moduli)
  1 0.089937 0.089652 -0.32 1.00 4 1 0.00 1.00
...
  7 0.144324 0.144502  0.12 1.00 7 3 0.41 0.59
...
 25 0.209741 0.209545 -0.09 1.00 1 4 0.05 0.95

Bulk Modulus=   0.3058

   c11    c22    c33    c23    c13    c12    c44    c55    c66
 0.52295 0.52295 0.52295 0.19721 0.19721 0.19721 0.16287 0.16287 0.16287

   d1     d2     d3
  0.47448  0.37700  0.48419

 loop# 4  rms error= 0.1473 %, changed by -.0000009 %
```

length of gradient vector= 0.000001 blamb= 0.000000

eigenvalues eigenvectors
0.84114 1.00 0.04
332.59760 -0.04 1.00

chisquare increased 2% by the following % changes in independent parameters
0.29 -0.04
0.00 0.05