Status

Overview

The benchmark Element0ktest is based on the work by Lejaeghere [**?**, **?**]. It includes the Elemental structures at zero Kelvin. The equation of state, i.e. equilibrium volume, bulk modulus and the derivative of the latter are compared the data calculated with the Wien2k code.

The test consists of

bin/Strcfiles	directory holding all structure files, yet without species information
bin/el_makedo	bash script which rebuilds the input data in the Cases directory
bin/specieslist	container of the species information for all elements
bin/splitspecies.f90	code to split up specieslist

To build up the test,

1. change the file specieslist so that the desired setup construction is selected for each element.

2. Adjust the variable PAWCMD in `src/el_makedo`.

3. execute

   ```
   bin/el_makedo
   ```

   This creates a new bash script `el_do_sample`. It also updates the setup information: The file `src/specieslist` is expanded into the files in the directory `bin/Speciesfiles`.

4. copy `el_do_sample` into `el_do`.

   ```
   cp el_do_sample el_do
   ```

   Unselect elements that shall not be studied by deleting or by commenting out the corresponding lines in the list.

5. construct a file `sample.cntl`.

   ```
   cp src/sample.cntl_strt sample.cntl
   ```

   This control file which will be used by all calculations. Take special care to remove `START=T`, when the restart files are present and if they shall be used.

6. perform the paw calculation by executing

   ```
   el_do -j 3 -- 1>out 2>&1 &
   ```

The calculation may take up to a few days. The calculations fill up the directory `Cases` which will contain one subdirectory for each element.

7. when the calculations are finished, update the result files `etot.dat`, `gap.dat` and `murn.in` with

   ```
   el_do -u
   ```

Experiences

For transition metals we need to set !POT:VAL0=0.
For Pd we had to increase !POT:POW from 3. to 5.