FHI-aims Cheat Sheet: Constrained Relaxation

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The cartesian coordinates of the atoms can be easily fixed by indicating it in the geometry.in file. However, for some problems, it is advantageous to constrain internal coordinates (distances, bond angles, or torsions). This can be achieved by using FHI-aims with PLUMED interface that allows for constrained geometry optimization. The executable provided by us already enables PLUMED. However, in general, the binary needs to be compiled separately using the Makefile.meta (more information can be found in section 1.4 of Chapter 1 of the FHI-aims Users' Guide).

How to begin?

1) Create a plumed.dat file and put it into the directory together with geometry.in and control.in. Now it's time to declare there the collective variables (CV). Collective variables like e.g. distances or torsions are constructed from the selected degrees of freedom. For each of the CVs the desired value must be specified together with the mode (UMBRELLA).
This is an example for a plumed.dat file:

```
DISTANCE LIST      7 8
ANGLE LIST       6 7 8
TORSION LIST  5 6 7 8          # CV type and list of its atoms
UMBRELLA CV 1 AT 2.09 KAPPA 1.
UMBRELLA CV 2 AT 2.35 KAPPA 1.
UMBRELLA CV 3 AT 1.57 KAPPA 1. # sampling type, index of the CV, value of the CV, spring constant
PRINT W_STRIDE 1               # grid for printing the output
ENDMETA
```

Diverse CVs can be defined. For a full list see the PLUMED manual. Note that PLUMED uses following units: bohr for distances, radians for angles and hartree/bohr^2 for the spring constant kappa.

2) Include following lines in the control.in file:

```
relax_geometry    bfgs_textbook 1.e-4
plumed_new .true.
```

3) Run it:

```
mpiexec -n 2 'FHI-aims binary' </dev/null > output
```

What do we get?

Besides the standard FHI-aims output file two additional files will be produced:

`PLUMED.OUT` - extensive description of the chosen CVs and settings
`COLVAR` - the time evolution of the CV

Visualize the relaxation, e.g. with `VMD`:

```
./create_xyz_movie.pl output > movie.xyz
vmd movie.xyz
```

You can check if the chosen constrain is fulfilled and how the relaxation progresses.

Attention!

These cheat sheets are not intended to substitute for reading the manuals of the programs involved and the original literature cited therein!
Have fun!