Short documentation of the input file syntax for atom-HF solver.

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The input template looks like this in example of a neon atom, where all the parameters that must be replaced are between low dash symbols "_". Only the text in **bold** contains input information, everything else is just comments.

```
Z Rmin Rmax Ngrid version sigma
_Z_ _Rmin_ _Rmax_ _Ngrid_ 1 _sigma_
xc_id(libxc_id or -1(LDA) -2(PBE))
_f1_ _f1w_ _f1par_
_f2_ _f2w_ 0
_f3_ _f3w_ 0
Non-local exchange:
_hyboverride_     (true to override hybrid libxc functional parameters)
_HFw_             (HF weigth)
_HFsrw_ _HFsrp_   (SR HF weigth and parameter)
Grid 0-equidistant 2-exponential 3-advanced_cubic
_grid_
Relativity(0-false, 1-nZORA, 2-ZORA)
_rel_
Spin polarised:
.false.
Number of shells:
3
List of shells: n l occupation
1 0 2.0d0
2 0 2.0d0
2 1 6.0d0
```

There is a script "script_list.py" that can generate and run inputs for you.
Description of the parameters:

_Z_	atomic number
Rmin	coordinate of the first grid point (everithing in Borh units (a.u.))
Rmax	coordinate of the last grid point
Ngrid	number of grid points
sigma	R_RMS of the nucleus. 0d0 in case of point-like nucleus
_f1_	id number of the first xc functional list of them available here: https://tddft.org/programs/libxc/functionals/. by using negative parameters -1 or -2 we use the build-in implementation of LDA (in case if -1) or PBE (in case if -2).
_f1w_	weight of the first xc functional.
f1par	0 if we leave all the default functional parameters defined in libxc. If we want to use different functional parameters, then this is the number of parameters defined for the functional in libxc and then should follow all the parameters in new lines.

_f2_	id number of the second xc functional.
_f2w_	weight of the second xc functional
_f3_	id number of the third xc functional
_f3w_	weight of the third xc functional
hyboverride	.true. if we want to override non-local exchange weigths, .false. if we will define them by ourselves.
HFw	weight of the exact HF exchange
HFsrw	weight of the short-range part of the HF exchange
HFsrp	range separation parameter
grid	type of the radial grid 0 - equidistant, 3 - cubic, 5 - 5-th order grid (5 is the best choice)
rel	relativity (0 – non, 1 - nZORA, 2 - ZORA)

Some examples of input files are available:

examples/ne-lda
examples/ne-pbe
examples/ne-hf
examples/ne-pbe0-a
examples/ne-pbe0-b (the same as ne-pbe0-a, just manually constructed PBE0)
examples/ne-lcblyp-a
examples/ne-lcblyp-b (the same as ne-lcblyp-a, just the short range parameter 0.33 passed to the libxc manualy)
examples/ne-lcblyp-c (the same as ne-lcblyp-a, just the non-local part is set manually)

Some examples with spin polarization (these results coincide with LDA and LSD configuratioins in: https://www.nist.gov/pml/atomic-reference-data-electronic-structure-calculations/atomic-reference-data-electronic-7-13):

examples/si-lda-a
examples/si-lda-b

To run the calculation the input file has to be passed like this:

./atomHF < examples/ne-lda

In the std output the solver gives useful information about functional like this:

```
 **********XC functional info:************
Libxc version: 5.1.5
 1-st XC functional number:          400
The functional 'LC version of BLYP' is an exchange-correlation functional, it belongs to the
'Hybrid GGA' family and is defined in the reference(s):
[1] Y. Tawada, T. Tsuneda, S. Yanagisawa, T. Yanai, and K. Hirao, J. Chem. Phys. 120, 8425 (2004)
 FUCTIONAL: LC version of BLYP Supports:            1 external parameters.
          0 . _omega default value:   0.33000000000000002       Range separation parameter

 **********Non-local exchange info************
 XC funcitional          400  contains non-local part.
 Fock exchange with weigth:    1.0000000000000000
 Fock SR exchange with weigth:   -1.0000000000000000       parameter:   0.33000000000000002
```