

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 weight)
_HFsrw_ HFsrp_    (SR HF weight 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:

<code>_Z_</code>	atomic number
<code>_Rmin_</code>	coordinate of the first grid point (everything in Bohr units (a.u.))
<code>_Rmax_</code>	coordinate of the last grid point
<code>_Ngrid_</code>	number of grid points
<code>_sigma_</code>	R_RMS of the nucleus. 0d0 in case of point-like nucleus
<code>_f1_</code>	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).
<code>_f1w_</code>	weight of the first xc functional.
<code>_f1par_</code>	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.

<code>_f2_</code>	id number of the second xc functional.
<code>_f2w_</code>	weight of the second xc functional
<code>_f3_</code>	id number of the third xc functional
<code>_f3w_</code>	weight of the third xc functional
<code>_hyboveride_</code>	.true. if we want to override non-local exchange weights, .false. if we will define them by ourselves.
<code>_HFw_</code>	weight of the exact HF exchange
<code>_HFsrw_</code>	weight of the short-range part of the HF exchange
<code>_HFsrp_</code>	range separation parameter
<code>_grid_</code>	type of the radial grid 0 - equidistant, 3 - cubic, 5 - 5-th order grid (5 is the best choice)
<code>_rel_</code>	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-lcblp-a
 examples/ne-lcblp-b (the same as ne-lcblp-a, just the short range parameter 0.33 passed to the libxc manually)
 examples/ne-lcblp-c (the same as ne-lcblp-a, just the non-local part is set manually)

Some examples with spin polarization (these results coincide with LDA and LSD configurations 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

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)
FUNCTIONAL: LC version of BLYP Supports:      1 external parameters.
      0 . _omega default value:  0.33000000000000002      Range separation parameter

*****Non-local exchange info*****
XC functional      400  contains non-local part.
Fock exchange with weight:  1.0000000000000000
Fock SR exchange with weight: -1.0000000000000000      parameter:  0.33000000000000002

```