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NCIPLOT4 MANUAL

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Theoretical background

The NonCovalent Interaction (NCI) index is a visualisation tool based on the density (ρ) and its derivatives. It enables the identification of non-covalent interactions from the reduced density gradient (RDG or s).

As highlighted in Figure 1, there is a crucial change in ρ between molecules due to the annihilation of the density gradient at these points, and so, in RDG.

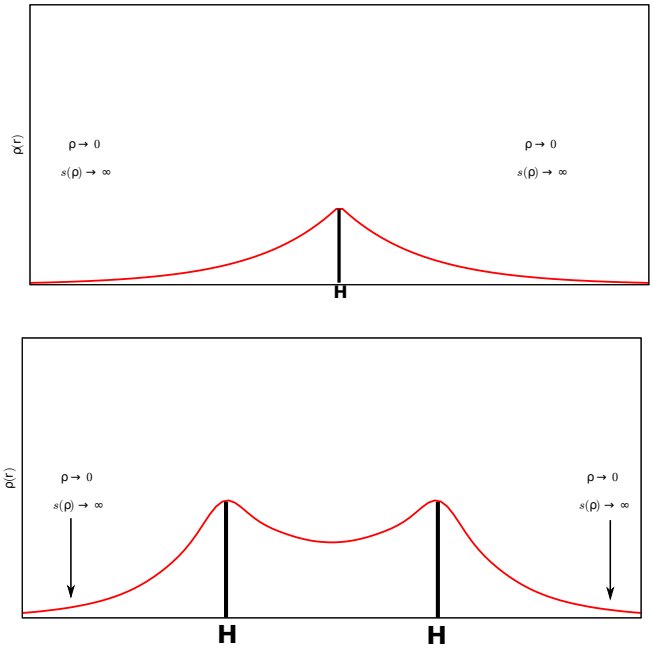

Figure 1: Schematic representation of the electron density (ρ) for the hydrogen atom (top) and for the H_2 molecule along the intermolecular axis(bottom). The reduced density gradient ($s(\rho)$) and (ρ) goes to infinity and zero far way from nuclear positions.

These variations lead to peaks when RDG is plotted against ρ. Figure 2 depicts RDG *vs* ρ for the benzene molecule and the benzene π-π dimer. The main difference between the monomer and the dimer is the appearance of steep peaks at low densities (Figure 2c).

To visualise the non-covalent interactions identified by the RDG *vs* ρ peaks, the 3D points whose values of RDG and ρ form the peaks

need to be found (Figure 2 b,d).

These interactions correspond to both favorable and unfavorable interactions. In order to differentiate between them, the sign of the second density Hessian eigenvalue (λ_2) times the density is implemented (sign$(\lambda_2)\rho$). This value is able to characterise the strength of the interactions by means of the density, and its nature thanks to the sign of the second eigenvalue. Attractive and repulsive interactions are identified as regions where $\lambda_2 < 0$ and $\lambda_2 > 0$, respectively. Weak van der Waals interactions by $\lambda_2 \approx 0$. To visualise these regions, it is often used a colour code based on sign$(\lambda_2)\rho$: blue for strong attractive interactions ($\lambda_2 < 0$), green for weak van der Waals interactions ($\lambda \approx 0$) and red for strong repulsive interactions ($\lambda_2 > 0$).

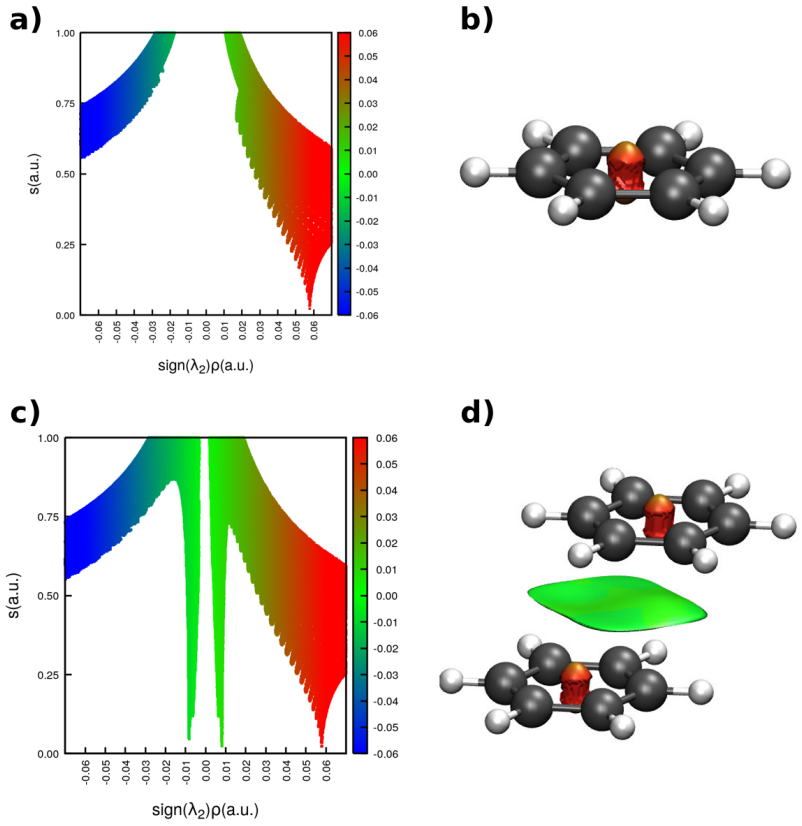

Figure 2: NCI analysis of the benzene dimer. RDG *vs* sign$(\lambda_2)\rho$ plots and RDG isosurfaces. A colour code based of sign$(\lambda_2)\rho$ was uses: -0.7 (blue) < 0.0 (green) < 0.7 (red). a) RDG *vs* sign$(\lambda_2)\rho$ for the benzene molecule. b) RDG isosurface for the monomer. c) RDG *vs* sign$(\lambda_2)\rho$ for the benzene dimer. d) RDG isosurface for the dimer.

Installing and running the program

To install NCIPLOT4, unpack or clone the contents of the distributionfrom https://github.com/juliacontrerasgarcia/nciplot. The following files should be found:

- LICENSE
- LOG
- README
- src_nciplot_4.0
- dat
- tests

The files LICENSE, LOG and README contain the GNU General Public License information, the latest modifications and compilation information respectively. The source code is located in the directory src_nciplot_4.0. The directory dat contains the atomic density files. Its path needs to be set during the compilation (see below). The directory test includes a large range of examples and scripts to execute them.

To compile the code go into the src_nciplot_4.0 subdirectory. Change the Makefile.inc to suit your compiler and flags and build the nciplot executables by executing the following commands:

```
make mrproper
make
```

To clean the object and module files,

```
make clean
```

To clean objects, modules and binaries,

```
make mrproper
```

NCIPLOT4 requires NCIPLOT_HOME environment variable to find the atomic density files contatined in the dat subdirectory. Set it to the absolute path to NCIPLOT:

```
export NCIPLOT_HOME=/home/xxx/nciplot/
```

You may add the previous lines to your .bashrc or .bash_aliases for convenience.

The code has been parallelised for shared-memory architectures using the OpenMP library. To use this feature, set the OME_NUM_THREADS environment variable to the number of cores:

```
export OMP_NUM_THREADS=4
```

If the compilation is completed successfully, an executable called nciplot is created. The code is invoked as follows:

```
nciplot input.file > ouput.file
```

The input

The input is keyword oriented, free-format, and the output is meant to be self-contained. Commentaries must be preceded by #. The following coding is used for variables:

- `r` stands for real.
- `x, y, z` stand for positions in space (real).
- `n` stands for integer.
- `name` stands for any character string.

Obligatory input

THE FIRST LINE MUST CONTAIN THE NUMBER OF FILES TO BE ANALISED.

Contrary to previous version, `NCIPLOT4` does accept multiple wfn and wfx files. Up to 100 files are supported by this version.

THE SECOND LINE MUST CONTAIN THE NAME OF THE MOLECULAR FILE. It accepts three different types of file format: xyz, wfn and wfx. They must have the following extensions depending on the desired calculation:

- `name.`**xyz** (Promolecular approximations) It requires an xyz file. Recommended for big systems.
- `name.`**wfn/wfx** wavefunction file in the AIMPAC WFN/WFX format (SCF calculation).

Optional keywords

- **1. RTHRES r**

  Add extra limits to the box (in Å). In order to ensure a correct cube in planar or linear cases, the code build a cubic box around the molecule, adding a minimun distance of 1.5 a.u. in all directions. This value is modified by `RTHRES`.

- **2. LIGAND n r**

  `n` is the number of the file (as written in the input) and `r` is a distance in Å.

  This option will only plot interactions around the molecule in the file `n` within a radius `r`

- **3. RADIUS x y z r**

  `x y z` determine the positions around which interactions are represented for a radius `r` (all in Å).

- **4. INTERMOLECULAR**

  This keyword triggers intermolecular interaction options.

  This option will turn off all the interactions where at least a fraction of the density comes from a single molecule. This enables only intermolecular interactions to be plotted, neglecting the intramolecular ones. The default is set so that an interaction is discarded if 0.95 of the density at the point comes from a single molecule. This value can be modified by the keyword (`INTERCUT`).

- **5. INTERCUT r_1, r_2**

  Cutoffs for intermolecularity definition. By default r1 and r2 are set to 0.95 and 0.75 respectively.

  .

- **6. ONAME name**

  `name` stands for the basic naming to be passed to the output file names. The `name` introduced will be always output in capital letters. By default, the root name of the structure file is taken.

- **7. INCREMENTS r_1 r_2 r_3**

  This option sets the increments along the x, y, z directions of the cube in Å. The default is set to 0.1, 0.1, 0.1.

- **8. OUTPUT n**

  `n` is an integer running from 1 to 3.

  - 1 will only print the .dat file.
  - 2 will only print the .cube files.
  - 3 will print all three output files [default]

- **9. FRAGMENT**

  ifile atom1, atom2, ..., atomn.

  Defining fragments from the .xyz files. `ifile` is the file label given by the input order and `atom` *n* is the atomic label in ifile

- **10. CUTOFFS r_1 r_2**

  Density (r_1) and RDG (r_2) cutoffs used in creating the dat file. The default cutoffs are 0.5 and 1.0 respectively.

- **11. CUTPLOT r_1 r_2**

  Density (r_1) and RDG (r_2) cutoffs used when creating the cube files. r_1 will set the cutoff for both the density and the RDG to be registered in the cube files, whereas r_2 will be used in the VMD script for the plotting of isosurfaces. The default values are:

  - In the promolecular case r_1=0.07 a.u., r_2=0.3 a.u.
  - In the SCF case: r_1=0.05 a.u., r_2=0.5.

- **12. ISORDG r**

  RDG isosurface used in the VMD script. This is equivalent to the parameter r_2 given in `CUTPLOT` (see above)

- **13. DGRID**

  Using grids for promolecular densities.

Computing properties withing NCI regions

- **14. INTEGRATE**

  Trigger the integration of properties.

- **15. RANGE**

  n

  $r_1$down $r_1$up

  $r_2$down $r_2$up

  $r_n$down $r_n$up

  Compute properties in n intervals of sign(λ_2)ρ.

  A lower and upper bounds are required for every interval. Interval limits should be written in different lines.

Multilevel grids

- **16. CG2FG n m_1 m_2, ...,m_{n-1}, m_n**

  Coarse grid to fine grid multi-level.

  n stands for the number of grids and m_1, m_2, ..., m_{n-1}, m_n=1 are the multiplicative factors that define the multilevel grids. This

factors must be integer number introduced in decreasing order $m_1 > m_2 > ... > m_{n-1} > m_n = 1$.

Notice that the size of the grid is eventually defined by the keyword `INCREMENTS`. Different grid steps may requires different multiplicative factors in CG2FG to achieve stability in the results. To easy the used of the multi-level grid approach, the grid step and the multilevel grid factors have been already optimized leading to the following keywords:

- **17. COARSE**

  Coarse multigrid option: CG2FG 4 8 4 2 1 and increments of 0.15 Å.

- **18. FINE**

  Fine multigrid option: CG2FG 4 12 8 4 1 and increments of 0.05 Å.

- **19. ULTRAFINE**

  Ultrafine multigrid option: CG2FG 4 24 16 8 1 and increments of 0.025 Å.

The output

The output (may) consist of 4 files:

- name.dat file collect ρ *vs* RDG (OUTPUT=1 or 3).
- name−grad.cube file with RDG (OUTPUT=2 or 3).
- name−dens.cube file with sign(λ_2)$\rho\times$ 100 (OUTPUT=2 or 3).
- name.vmd is a script for the visualization of the results in VMD.

The structure of the output is similar to the previous version of the code:

```
 # ----------------- NCIPLOT -----------------------
# --- PLOTTING NON COVALENT INTERACTION REGIONS ----
# ---             E.R. Johnson                  ----
# ---          J. Contreras-Garcia              ----
# ----------    Duke University         ------------
#
# ---             A. de la Roza                  ---
# --------- University of California Merced --------
#
# ---               R. A. Boto                   ---
# ---                 C. Quan                     --
# --------  UniversitÃl' Pierre et Marie Curie -------
# -------------------------------------------------
# ---              Please cite                  ----
# --J. Am. Chem. Soc., 2010, 132 (18), pp 6498âĂŞ6506-
# -------------------------------------------------
# -------------------------------------------------
# ---     Contributions for the wfn properties  ----
# ---      from H. L. Schmider are acknowledged  ---
# -------------------------------------------------
# -------------------------------------------------
# ---     Contributions for the wfx reader      ----
# ---      from Dave Arias are acknowledged      ---
```

```
 # ------------------------------------------------
 #
 # Start -- 2020.06.07, 08:45:59.333

+ Read density file : /home/roberto/src/nciplot-intermolecular_wfn/dat/h__lda.wfc
  Log grid (r = a*e^(b*x)) with a =   2.4788E-03, b =   2.0000E-03
  Num. grid points =  4392, rmax (bohr) =    16.1513
  Integrated charge =           0.99999998
  El. conf. :  1S(1)

+ Read density file : /home/roberto/src/nciplot-intermolecular_wfn/dat/c__lda.wfc
  Log grid (r = a*e^(b*x)) with a =   4.1313E-04, b =   2.0000E-03
  Num. grid points =  5326, rmax (bohr) =    17.4308
  Integrated charge =           5.99999996
+ Read density file : /home/roberto/src/nciplot-intermolecular_wfn/dat/n__lda.wfc
  Log grid (r = a*e^(b*x)) with a =   3.5411E-04, b =   2.0000E-03
  Num. grid points =  5343, rmax (bohr) =    15.4574
  Integrated charge =           6.99999996
  El. conf. :  1S(2) 2S(2) 2P(3)

+ Read density file : /home/roberto/src/nciplot-intermolecular_wfn/dat/o__lda.wfc
  Log grid (r = a*e^(b*x)) with a =   3.0984E-04, b =   2.0000E-03
  Num. grid points =  5358, rmax (bohr) =    13.9372
  Integrated charge =           7.99999996
  El. conf. :  1S(2) 2S(2) 2P(4)

-----------------------------------------------------
      INPUT INFORMATION:
-----------------------------------------------------

      MIND YOU
      RUNNING IN PROMOLECULAR MODE


-----------------------------------------------------
      Calculation details:
-----------------------------------------------------
RHO  THRESHOLD   (au): 0.50
RDG  THRESHOLD   (au): 1.00

-----------------------------------------------------
      Writing output in the following units:
-----------------------------------------------------
```

```
 Sign(lambda2)xDensity x Reduced Density Gradient    = AT.dat

 Reduced Density Gradient,RDG      = AT-grad.cube
 Sign(lambda2)xDensity,LS          = AT-dens.cube
 VMD script                        = AT.vmd
```

When multilevel grip option is trigger, the features of each grid are printed as:

```
-----------------------------------------------------
      Operating grid and increments: Grid-1
-----------------------------------------------------
 x0,y0,z0  =   -11.7843    -3.0798    -6.9277
 x1,y1,z1  =    13.8483     3.2251     6.3277
 ix,iy,iz  =  1.13    1.13    1.13
 nx,ny,nz  =   23       6      12

 Time for computing density & RDG =   0.00 secs
  0.00% of small boxes are removed.


-----------------------------------------------------
      Operating grid and increments: Grid-2
-----------------------------------------------------
 x0,y0,z0  =   -11.7843    -3.0798    -6.9277
 x1,y1,z1  =    13.8483     3.2251     6.3277
 ix,iy,iz  =  0.76    0.76    0.76
 nx,ny,nz  =   34       9      18

 Time for computing density & RDG =   0.01 secs
  0.00% of small boxes are removed.


-----------------------------------------------------
      Operating grid and increments: Grid-3
-----------------------------------------------------
 x0,y0,z0  =   -11.7843    -3.0798    -6.9277
 x1,y1,z1  =    13.8483     3.2251     6.3277
 nx,ny,nz  =   68      17      36

 Time for computing density & RDG =   0.06 secs
```

```
  0.06% of small boxes are removed.


-----------------------------------------------------
      Operating grid and increments: Grid-4
-----------------------------------------------------
 x0,y0,z0  =   -11.7843    -3.0798    -6.9277
 x1,y1,z1  =    13.8483     3.2251     6.3277
 ix,iy,iz  =  0.05    0.05    0.05
 nx,ny,nz  =  543     134     281

 Time for computing density & RDG =  30.52 secs
 58.43% of small boxes are removed.
 Time for writing outputs =  45.38 secs
 59.49% of small boxes removed for promolecular integration
```

The last bunch of information is related to the integration of ρ^n and sign$(\lambda_2)\rho^n$ within the NCI regions and over their boundaries:

$\int_{\Omega_{NCI}} \rho^n((\mathbf{r})d\mathbf{r}, \quad n = 0, 1, 1.5, 2, 2.5, 3, 4/3, 5/3$

$\int_{\Omega_{NCI}} sign(\lambda_2)\rho^n(\mathbf{r})d\mathbf{r} \quad n = 0, 1, 1.5, 2, 2.5, 3, 4/3, 5/3$

It is worth mentioning that the volume of Ω_{NCI} is defined by the integral $\rho^{n=0}$

```
-----------------------------------------------------------------------

                    INTEGRATION DATA
 ------------------------------------------------------------------------
 Integration  over the volumes of rho^n
-------------------------------------------------------------------------
 n=1.0           :       81.78751055
 n=1.5           :       32.71905205
 n=2.0           :       14.92576555
 n=2.5           :        7.52272297
 n=3.0           :        4.08744955
 n=4/3           :       43.71246189
 n=5/3           :       24.89093300
 Volume          :      862.16226131
```

```
 rho-sum_i rho_i :        0.14776508

-----------------------------------------------------------------------
 Integration  over the volumes of sign(lambda2)(rho)^n
-----------------------------------------------------------------------
 n=1.0           :      -38.78097498
 n=1.5           :      -21.57715460
 n=2.0           :      -11.75189302
 n=2.5           :       -6.56180728
 n=3.0           :       -3.78238954
 n=4/3           :      -26.48446142
 n=5/3           :      -17.60409566
-----------------------------------------------------------------------
 Integration  over the areas of rho^n
-----------------------------------------------------------------------
 n=1.0           :       52.68576805
 n=1.5           :       33.08255593
 n=2.0           :       23.80536956
 n=2.5           :       17.72600807
 n=3.0           :       13.31834056
 n=4/3           :       37.69490189
 n=5/3           :       29.42766077
 Area            :      552.43261501
 rho-sum_i rho_i :        0.23567316
-----------------------------------------------------------------------
   Time for integration =  62.22 secs
End -- 2020.06.07, 08:48:21.087
```

Examples

In all cases 2D and 3D pictures have been obtained by applying the VMD script from the calculation. The background and atom colours were edited.

Number of files

In this case, different options are possible. If all the interactions are wanted, molecules are introduced in a unique file or two separate files:

```
1
24_Benzene-Benzene_pi-pi.xyz
FINE
```

```
2
24_Benzene-Benzene_pi-pi_monomerA.xyz
24_Benzene-Benzene_pi-pi_monomerB.xyz
FINE
```

In both cases the same result is obtained:

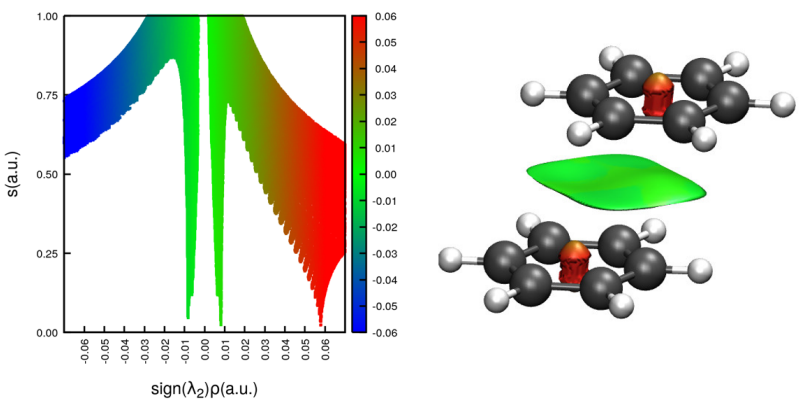

Figure 3: NCI analysis of the benzene dimer. (Left) RDG *vs* $sign(\lambda_2)\rho$ plot. (Right) 0.5 RDG isosurface. Colour code: -0.05(blue), 0.00(green), 0.05(red)

Computing properties within the NCI regions

In the following example the intermolecular interactions in the water dimer are analysed. To compute properties, NCI regions are built from water monomers wavefunctions as contained in the files A22_Water-Water.wfx and B22_Water-Water.wfx.

```
2
A22_Water-Water.wfx
B22_Water-Water.wfx
FINE
OUTPUT 3
INTEGRATE
INTERMOLECULAR
INTERCUT 0.75 0.75
```

The first command, 2, tells the program that two files are to be read: A22_Water-Water.wfx and B22_Water-Water.wfx. The keyword FINE defines the multigrid level: 4 12 8 4 1, and grid increments 0.05, 0.05, 0.05. That is, four grids are going to be used with step sizes: 0.05x12=0.6, 0.05x8=0.4, 0.05x4=0.2 and 0.05x1=0.05. `OUTPUT 3` generates four output file: A22_Water-Water.dat with sign$(\lambda_2)rho$ vs RDG, sign$(\lambda_2)\rho$ and ρ Gaussian cube files: A22_Water-Water-grad.cube A22_Water-Water-dens.cube respectively, and a VMD script to plot them: example.vmd

`INTEGRATE` triggers the computation of properties within the NCI regions.

`INTERMOLECULAR` and `INTERCUT` defines intermolecular interactions as defined above using the parameter 0.75 and 0.75.

This above input could be also written as:

```
2
A22_Water-Water.wfx
B22_Water-Water.wfx
CG2FG 4 12 8 4 1
INCREMENTS 0.05 0.05 0.05
OUTPUT 3
INTEGRATE
INTERMOLECULAR
INTERCUT 0.75 0.75
```

Similar to the previous versions of the code, .cube and .dat files allow to visualised NCI interactions. As shown in Figure 4, the

hydrogen bonding in the water dimer is visualised as a lenticular isosurface between the water molecules. When RDG is plotted against $sign(\lambda_2)\rho$, a dip between 0.02 and 0.03 a.u.

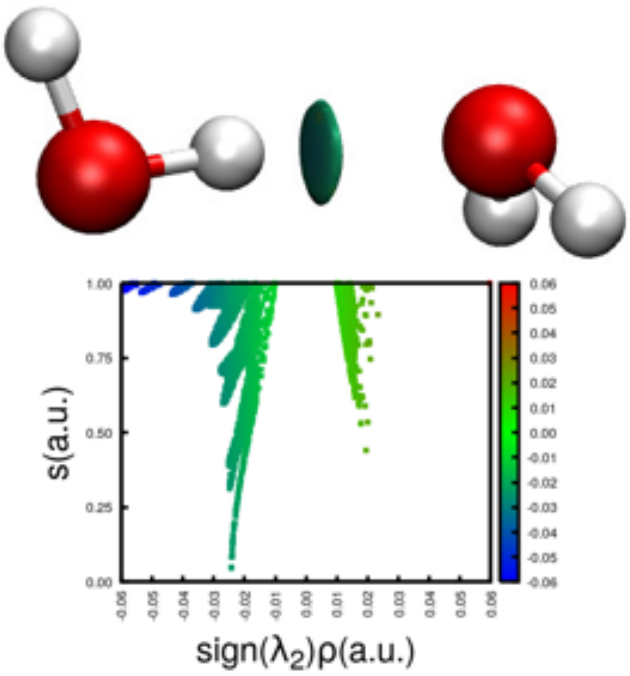

Figure 4: NCI analysis of the water dimer. (Top) 0.5 RDG isosurface. ((Botton) RDG *vs* $sign(\lambda_2)\rho$ plot Colour code: -0.05(blue), 0.00(green), 0.05(red)

Beyond the qualitative analysis, quantification of non-covalent interactions are possible with NCIPLOT4. Integration over the NCI regions is given in three separated blocks. In the first block integrals of ρ^n are printed:

```
-----------------------------------------------------------------
 Integration  over the volumes of rho^n
-----------------------------------------------------------------
 n=1.0           :        0.00976859
 n=1.5           :        0.00114406
 n=2.0           :        0.00013489
 n=2.5           :        0.00001601
 n=3.0           :        0.00000191
 n=4/3           :        0.00233997
 n=5/3           :        0.00056217
 Volume          :        0.72628959
 rho-sum_i rho_i :        0.00000134
```

Next, integrals of $sign(\lambda_2)\rho$ are printed.

```
-----------------------------------------------------------------
 Integration  over the volumes of sign(lambda2)(rho)^n
-----------------------------------------------------------------
 n=1.0           :        0.00571364
 n=1.5           :        0.00065746
 n=2.0           :        0.00007188
 n=2.5           :        0.00000782
 n=3.0           :        0.00000084
 n=4/3           :        0.00137594
 n=5/3           :        0.00031544
```

In the third block, integrals over the boundaries of the NCI region are printed:

```
-----------------------------------------------------------------
 Integration  over the areas of rho^n
-----------------------------------------------------------------
 n=1.0           :        0.09203179
 n=1.5           :        0.01089971
 n=2.0           :        0.00130481
 n=2.5           :        0.00015793
 n=3.0           :        0.00001933
 n=4/3           :        0.02216897
 n=5/3           :        0.00536540
 Area            :        6.76716841
 rho-sum_i rho_i :        0.00001298
-----------------------------------------------------------------
```

Protein-Ligand interaction

In this example, the interaction between the protein 2v5x and a ligand is studied. The structure of the protein and the ligand is contained in the files 2v5x-within5.xyz and 2v5x-ligand.xyz respectively.

```
2                  # Number of files to be read
2v5x-within5.xyz   # Protein structure
```

```
2v5x-ligand.xyz     # Ligand structure
LIGAND 2 4.         # Only interactions at 4 Angstroms from the ligand  are analysed
ONAME 2v5x          # Output files name
FINE                # Multigrid and increments definition.
RANGE 3             # Integration is performed in three ranges.
-0.1 -0.02
-0.02 0.02
0.02 0.1
```

To remove the intramolecular interactions within the protein the `LIGAND` keyword is used (See Figure 5). Only interactions at 4 Åaround the ligand, given by the file number 2. The grid increments and multigrid level is given by the FINE keyword: CG2FG 4 12 8 4 1 and reference increments of 0.05.

Sometimes it is interesting to compute properties in the attractive ($sign(\lambda_2)\rho < 0$), van der Waals ($sign(\lambda_2)\rho \approx 0$) and repulsive ($sign(\lambda_2)\rho > 0$) regions separately. This is done with the keyword RANGE. In the example above, integration will be computed in three ranges:

- Range 1: -0.01 < $sign(\lambda_2)\rho$ < -0.02.
- Range 2: -0.02 < $sign(\lambda_2)\rho$ < 0.02.
- Range 3: 0.02 < $sign(\lambda_2)\rho$ < 0.01.

Integration of ρ^n and $(\lambda_2)\rho^n$ are printed for each block.

```
-----------------------------------------------------------------
 Integration  over the volumes of rho^n
-----------------------------------------------------------------
 n=1.0           :        2.97614936
 n=1.5           :        0.58755898
 n=2.0           :        0.11949129
 n=2.5           :        0.02506085
 n=3.0           :        0.00542289
 n=4/3           :        1.00690144
 n=5/3           :        0.34509889
 Volume          :       82.88980295
 rho-sum_i rho_i :        0.00118474
 -----------------------------------------------------------------
```

In all cases 3D pictures have been obtained by directly applying the VMD script from the calculation. The lines defining the cube edges have also been highlighted when appropriate.

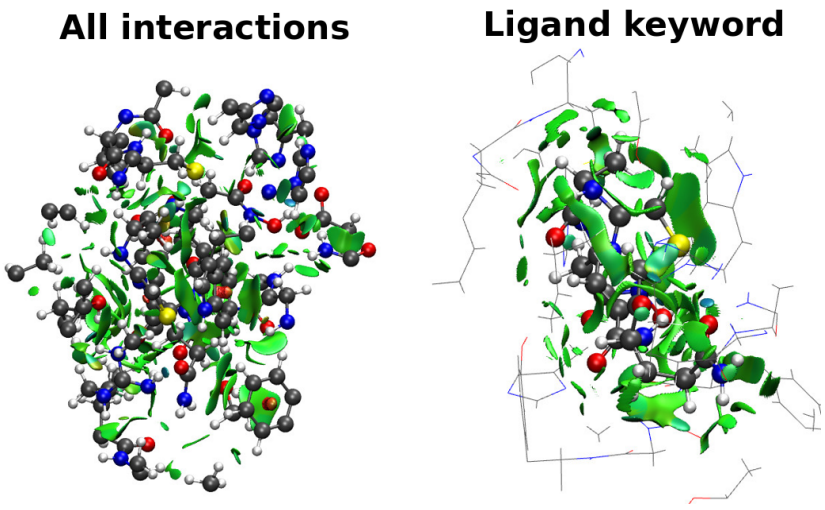

Figure 5: NCI analysis of the 2v5x-ligand interaction. Comparison of the isosurfances obtained without the `LIGAND`(left) keyword and with it (right). 0.3 RDG isosurface. Colour code: -0.07(blue), 0.00(green), 0.07(red)

Choosing the interactions

The adenine-thymine complex is small system where several non-covalent interaction are at play: hydrogen bonds, van der Waals interactions and steric clashes. This can be easily revealed by a standard calculation:

```
1
AT.xyz
INTEGRATE
ULTRAFINE
```

In this case we use the ULTRAFINE keyword, which sets the multilevel grids 4 12 8 4 1, and a reference grid increments 0.025 Å.

Steric clashes can be ruled out by the `INTERMOLECULAR` keyword. To use `INTERMOLECULAR`, adenine and thymine structures have to be input in separate files:

```
 2
A.xyz
T.xyz
INTEGRATE
INTERMOLECULAR
ULTRAFINE
ONAME AT
```

By default, the code takes the root name of the fist .xyz file to, A in this example, to name the output files. To avoid this behavior the keyword `ONAME` is used.

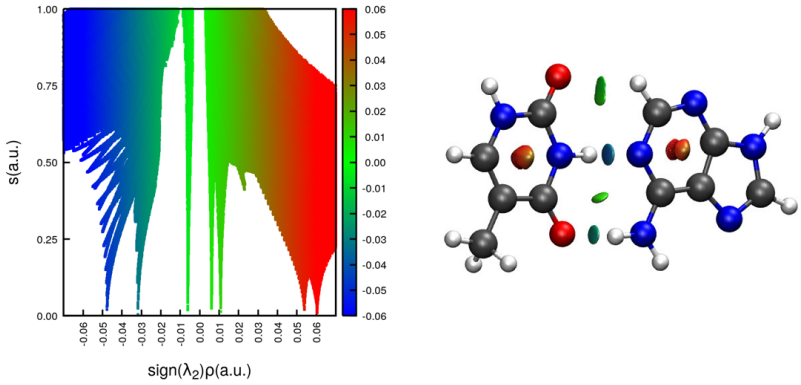

Figure 6: NCI analysis of the adenine-thymine complex. (Left) RDG *vs* $sign(\lambda_2)\rho$ plot. (Right) 0.5 RDG isosurface. Colour code: -0.05(blue), 0.00(green), 0.05(red)

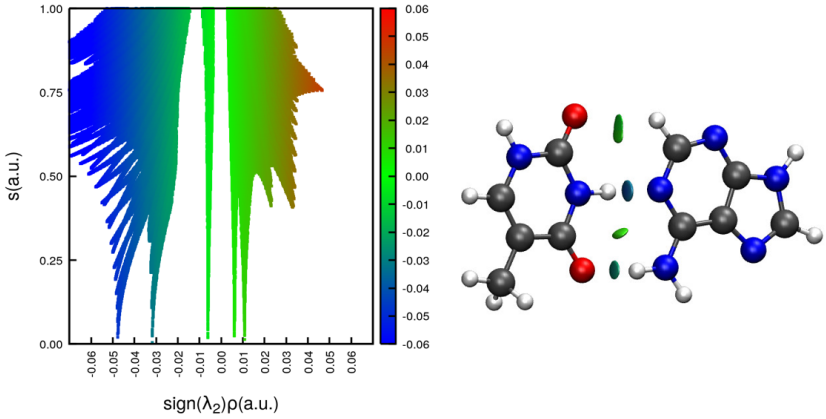

Figure 7: Intermolecular interactions in the adenine-thymine complex. (Left) RDG *vs* $sign(\lambda_2)\rho$ plot. (Right) 0.5 RDG isosurface. Colour code: -0.05(blue), 0.00(green), 0.05(red)

Sometimes, it is interesting to split non-covalent interactions in real space. This is possible using the `RADIUS` keyword.

```
1
AT.xyz
RADIUS -1.0285 -0.011 0.5 1.0
INTEGRATE
FINE
```

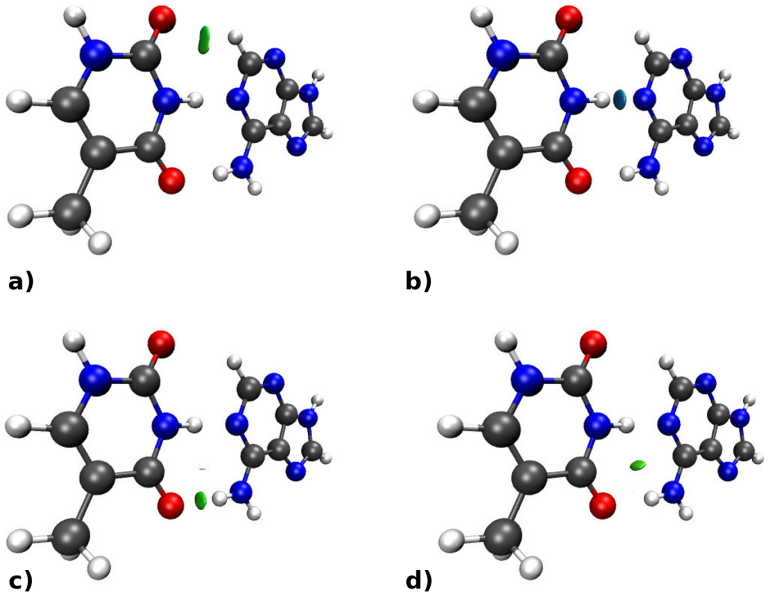

Figure 8: `RADIUS` kewyword.NCI analysis of the adenine-thymine complex. The value of RADIUS are: a) -0.185 -0.017 -2.756 1.5; b) -0.537 -0.027 -0.593 1.0; c) 0.40 -0.048 1.789 1.0; d) -1.0285 -0.011 0.5 1.0.

Useful scripts

Using the VMD script

The program generates a script for visualization of the result under the `name.vmd`. This script can be loaded in VMD. After entering the working directory, the script will automatically generate an NCI picture with a RDG cutoff as specified by the keyword `PLOTCUT` (otherwise, a default is used).

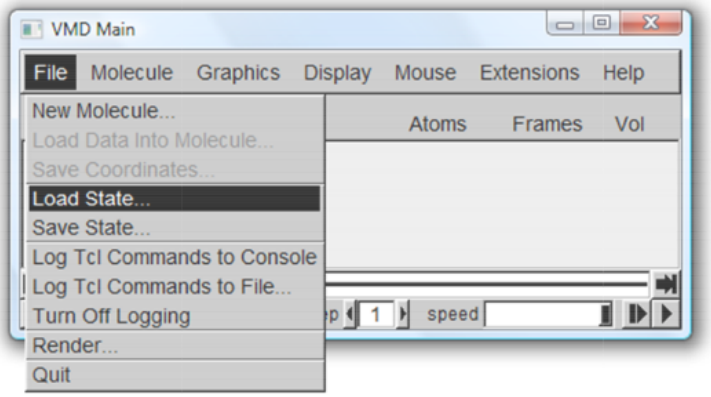

Figure 9: Image caption of the VMD dashboard.

The script is as follows:

In case the user wants to change it, the main options have been highlighted in red:

- `name-dens.cube`: name of the density cube file
- `name-grad.cube`: name of the gradient cube file
- 0.30000: value of RDG isosurface
- -4.0000 4.0000 where this is 100 times the value of rhoplot

In order to generate figures ready of publication quality, the background needs to be colour in white. This can be done by going to the GRAPHICS slash, and select COLORS.

Plotting RDG vs sign(λ_2)ρ with Gnuplot

All the plots of RDG vs sign(λ_2)ρ have been generated with the following script:

```
  # Gnuplot script for mapping NCI color code over NCI diagrams, by R.A.Boto
set terminal pngcairo size 1000,1000 enhanced font 'Helvetica,20'
set encoding iso_8859_1
set output 'AT_2d.png'
set key
set ylabel 's(a.u.)' font "Helvetica, 30"
set xlabel 'sign({/Symbol l}_2){/Symbol r}(a.u.)' font "Helvetica, 30"
set pm3d map
# Define a color gradient palette used by pm3d
set palette defined (-0.07 "blue",0.00 "green", 0.07 "red")
set format y "% .2f"
set format x "% .2f"
set format cb "% -.2f"
set border lw 4
set xtic  -0.06,0.01,0.06 nomirror rotate font "Helvetica"
set ytic   0.0,0.25,1.0 nomirror font "Helvetica"
# set the color bar tics
set cbtic  -0.06,0.01,0.06 nomirror font "Helvetica"
set xrange [-0.07:0.07]
set yrange [0.0:1.0]
# set the range of values which are colored using the current palette
set cbrange [-0.06:0.06]
plot 'AT.dat' u 1:2:1 w p lw 6 palette t ''
```