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NCIPLOT4.4 MANUAL

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List of Keywords

1 RTHRES r 9
2 LIGAND n r 10
3 RADIUS x y z r 10
4 INTERMOLECULAR 10
5 INTERMOL_CUTOFF γ_{ref} 10
6 ONAME name 10
7 INCREMENTS r_1 r_2 r_3 10
8 OUTPUT n 10
9 CUBE_PARAM x_0 y_0 z_0 x_1 y_1 z_1 11
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18 NCIENERGY 12
19 SUPRA 12
20 CG2FG n m_1 m_2, ...,m_{n-1}, m_n 12
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Theoretical background

The Non-Covalent 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.

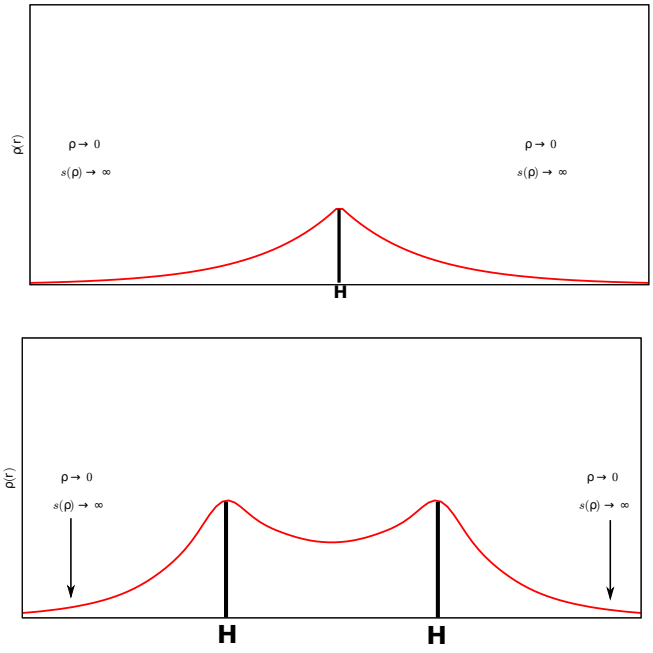

Figure 1: Schematic representation of the electron density (ρ) for the hydrogen atom (top) and for the H_2 molecule along the intermolecular axis(bottom). The reduced density gradient ($s(\rho)$) and (ρ) goes to infinity and zero far way from nuclear positions.

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 ($\lambda_2 > 0$).

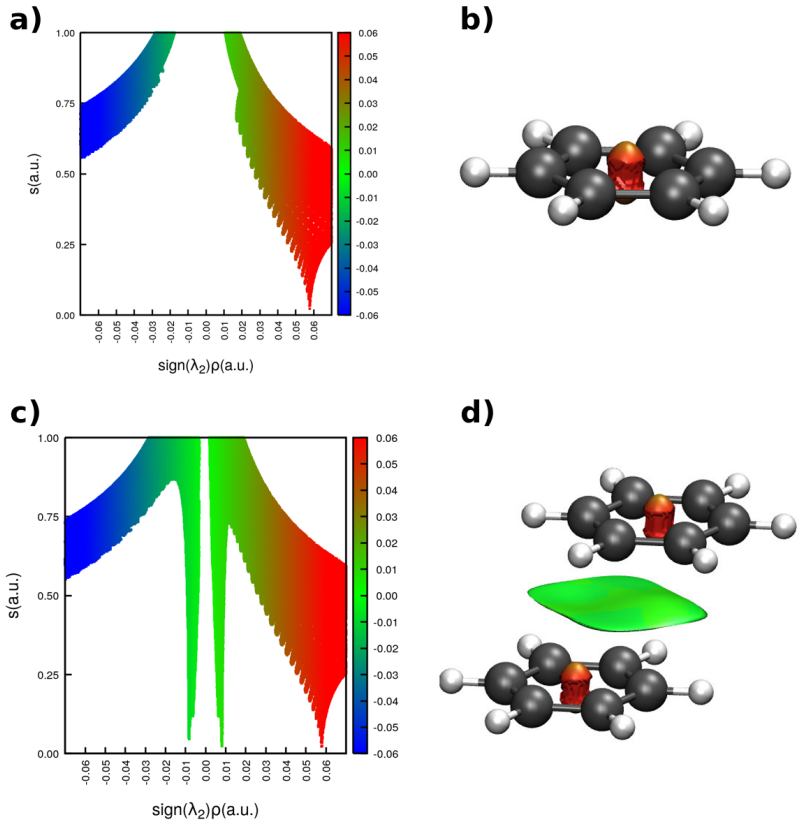

Figure 2: NCI analysis of the benzene dimer. RDG *vs* sign$(\lambda_2)\rho$ plots and RDG isosurfaces. A colour code based of sign$(\lambda_2)\rho$ was uses: -0.7 (blue) < 0.0 (green) < 0.7 (red). a) RDG *vs* sign$(\lambda_2)\rho$ for the benzene molecule. b) RDG isosurface for the monomer. c) RDG *vs* 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 distribution from https://github.com/juliacontrerasgarcia/nciplot. Alternatively, the newest version can be downloaded from https://github.com/kzator/NCIPLOT-4.4. The following files should be found:

- LICENSE
- README
- src_nciplot_4.4
- scripts
- dat

The files LICENSE and README contain the GNU General Public License information, the latest modifications, and compilation information, respectively.

To compile the code, navigate into the NCIPLOT-4.4 directory. Change 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 contained 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 ḃashrc 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. Comments 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 ANALYSED.

`NCIPLOT4` can support up to 100 wfn and wfx files.

THE SECOND LINE MUST CONTAIN THE NAME OF THE MOLECULAR FILE. There are four different acceptable types of file formats: xyz, cube, wfn, and wfx. They must have the following extensions depending on the desired calculation:

- `name.`**xyz** (will use the promolecular approximation). Recommended for big systems.
- `name.`**wfn/wfx** wavefunction file in the AIMPAC WFN/WFX format (SCF calculation).
- `name.`**cube** density file in the cube format. If, by any reason, the .cube files present negative density values, they will be treated as absolute values.

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 builds a cubic box around the

molecule, adding a minimum 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 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 0.85 of the density at the point comes from a single molecule. This value can be modified by the keyword (`INTERMOL_CUTOFF`).

- **5. INTERMOL_CUTOFF** γ_{ref}

  Cut-off specifying a maximum fractional contribution of each monomeric density to total density in the intermolecular region - the definition of intermolecular. By default, it is set to 0.85.

- **6. ONAME name**

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

- **7. INCREMENTS** $\mathbf{r}_1$ $\mathbf{r}_2$ $\mathbf{r}_3$

  This option sets the increments along the x, y, and 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. CUBE_PARAM x_0 y_0 z_0 x_1 y_1 z_1**

  This option will set the cube within which NCI is analysed as going from Cartesian coordinate (x_0 y_0 z_0 x_1 y_1 z_1) (all in Å)

  The default is produced in terms of molecular coordinates. In order to ensure a correct cube in planar or linear cases, a minimum distance of +/- 1.5 a.u. is added to the axes in all directions. This value can be modified by the keyword `RTHRES`

- **10. 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

- **11. RGD_CUTOFF s_1 s_2**

  RDG (r_2) cut-off for the NCI interaction region, also used in .dat and .cube files, and the integration. r_2 is the RDG cut-off used in VMD for region plotting. The default cut-offs are 1.0 and 0.5, respectively.

- **12. DENS_CUTOFF r_1**

  Density (r_1) cut-off deciding the integration region. It should be equal to outer values for range integration. The default value is:

  - In the promolecular case r_1=0.07 a.u.
  - In the SCF case: r_1=0.05 a.u.

- **13. DGRID**

  Using grids for promolecular densities.

- **14. DENSWEIGHT w_1, w_2, ..., w_n**

  Customises the relative weighting of WFN electron density inputs into the total density, ρ. Currently only available for .wfn files.

- **15. CLUSTERING**

  Identify non-covalent interaction regions based on the underlying bond critical points, thus separating the individual interactions spatially. NCICLUSTER uses the output cube files of NCIPLOT and performs integration of the regions using the matching input parameters. Watch out, NCICLUSTER depends on the scikit-learn library that needs to be installed separately ahead of the run.

Computing properties within NCI regions

- **16. INTEGRATE**

  Trigger the integration of NCI regions.

- **17. RANGE n**

  $r_{large,1}$ $r_{small,1}$
  $r_{small,1}$ $r_{small,2}$
  $r_{small,n}$ $r_{large,n}$
  Compute properties in n intervals of sign(λ_2)ρ.

  Lower and upper bounds are required for every interval. Interval limits should be written on different lines.

- **18. NCIENERGY**

  Triggers the calculation of energies for the NCI regions. There are distinct equations for sigma holes and other interactions, for promolecular and WFN modes, hence the exact energy estimations might differ. When CLUSTER is also selected, each found cluster gets an energy estimate of its own. To run properly, it requires selection of default parameters to work due to its sensitivity to the size of the NCI region.

- **19. SUPRA**

  Triggers the supramolecular mode - the calculation of energies now uses different equations better suited for larger complexes. It is compatible with promolecular mode with and without the CLUSTER keyword, however since these equations need to be necessarily extensive for the latter, their functional form is a little bit different, giving the energy estimates with slightly (+1 kJ/mol) higher error. It is not yet available for the WFN mode.

Multilevel grids

- **20. 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 require different multiplicative factors in CG2FG to achieve stability in the results. To

ease the use of the multi-level grid approach, the grid step and the multilevel grid factors have already been optimised, leading to the following keywords:

- ***21.* COARSE**

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

- ***22.* FINE**

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

- ***23.* 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                     --
 # --------  Université Pierre et Marie Curie -------
 # ------------------------------------------------
 # ---              Please cite                  ----
 # --J. Am. Chem. Soc., 2010, 132 (18), pp 6498-6506-
 # ------------------------------------------------
 # ------------------------------------------------
 # ---     Contributions for the wfn properties  ----
 # ---      from H. L. Schmider are acknowledged  ---
 # ------------------------------------------------
 # ------------------------------------------------
 # ---     Contributions for the wfx reader      ----
 # ---      from Dave Arias are acknowledged      ---
 # ------------------------------------------------
```

```
 # -------------------------------------------------
 # ---     Contributions for the integration --------
 # ---      algorithms from Erna Wieduwilt    -------
 # ---             are acknowledged           -------
 # -------------------------------------------------
 # -------------------------------------------------
 # ---   Contributions for the clustering and    ----
 # ---  energy algorithms from Katarzyna Zator   ----
 # ---             are acknowledged             ----
 # -------------------------------------------------
 #
 # Start -- 2025.07.17, 22:42:18.267

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

      MIND YOU
      RUNNING IN PROMOLECULAR MODE

 RHO  THRESHOLD   (au): 0.20
 RDG  THRESHOLD   (au): 1.00
 INTERMOLECULARITY THRESHOLD : 0.85
```

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

-------------------------------------------------
      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

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

```
      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

-------------------------------------------------
      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 writing outputs =  45.38 secs
```

More information about the calculation can be obtained when using the VERBOSE keyword.

The last piece of information is related to the integration of ρ^n and $\text{sign}(\lambda_2)\rho^n$ within the NCI regions and over their boundaries, and Volume of Ω_{NCI} is defined by the integral $\rho^{n=0}$:

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

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

```
-----------------------------------------------------------------------
                     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 by cubes =   0.40 secs
```

The integration can be further divided by use of RANGE keyword, whereby the integration occurs in regions constrained by the values specified. The default values are: -0.2/-0.02, -0.02/0.02, and 0.02/0.2.

When CLUSTERING keyword is used, additional range integration (with the ranges specified or default) over the individual clusters takes place the values are printed below.

Examples

In all cases 2D pictures were obtained with gnuplot and 3D pictures - with a VMD script from the calculation. The background (to white, no depth cueing) and atom colours were edited (carbon to black).

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. In both cases, the same result is obtained.

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

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

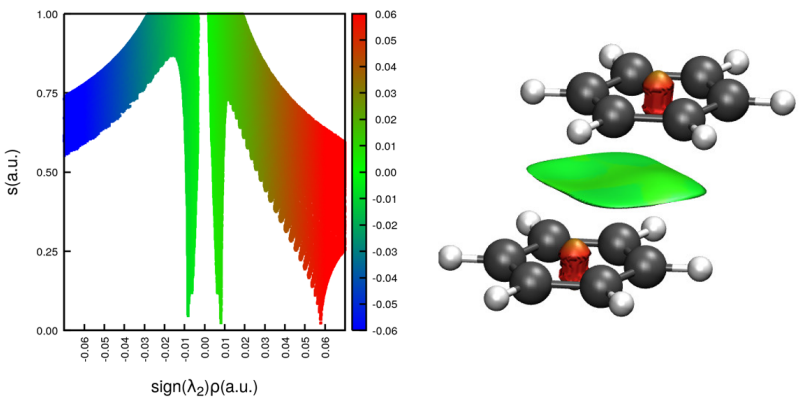

Figure 3: NCI analysis of the benzene dimer. (Left) RDG *vs* $sign(\lambda_2)\rho$ plot. (Right) 0.5 RDG isosurface. Colour code: -0.05(blue), 0.00(green), 0.05(red)

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.wfn and B22_Water-Water.wfn.

```
2
A22_Water-Water.wfn
B22_Water-Water.wfn
FINE
OUTPUT 3
INTEGRATE
INTERMOLECULAR
INTERMOL_CUTOFF 0.85
```

The first command, 2, tells the program that two files are to be read: A22_Water-Water.wfn and B22_Water-Water.wfn. 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(λ_2)*rho* vs RDG, sign(λ_2)ρ and ρ Gaussian cube files: A22_Water-Water-grad.cube A22_Water-Water-dens.cube respectively, and a VMD script to plot them: A22_Water-Water.vmd

INTEGRATE triggers the computation of properties within the NCI regions.

INTERMOLECULAR and INTERMOL_CUTOFF define intermolecular interactions as defined above using the parameter 0.85.

Similar to the previous versions of the code, .cube and .dat files allow for visualising NCI interactions. As shown in Figure 4, the hydrogen bonding in the water dimer is visualised as a lentil-shaped isosurface between the water molecules. When RDG is plotted against $sign(\lambda_2)\rho$, a dip between 0.02 and 0.03 a.u.

Beyond the qualitative analysis, quantification of non-covalent interactions is possible with NCIPLOT4. Integration over the NCI regions is given in three separate 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
```

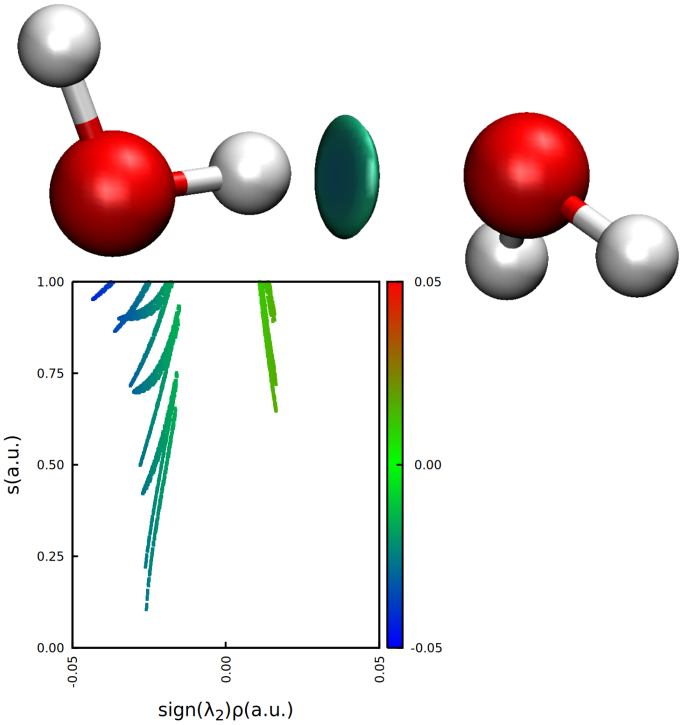

Figure 4: NCI analysis of the water dimer. (Top) 0.3 RDG isosurface. ((Bottom) RDG *vs* $sign(\lambda_2)\rho$ plot. Colour code: -0.05(blue), 0.00(green), 0.05(red)

```
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
```

Second block contains integrals of $sign(\lambda_2)\rho$, and the third block has integrals over the boundaries of the NCI region.

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.
-0.2 -0.02
-0.02 0.02
0.02 0.2
```

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 are given by the FINE keyword: CG2FG 4 12 8 4 1 and reference increments of 0.05.

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: -0.20 < $sign(\lambda_2)\rho$ < -0.02.
- Range 2: -0.02 < $sign(\lambda_2)\rho$ < 0.02.
- Range 3: 0.02 < $sign(\lambda_2)\rho$ < 0.20.

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

```
-------------------------------------------------------------------
               RANGE INTEGRATION DATA
-------------------------------------------------------------------

-------------------------------------------------------------------
 Interval        :       -0.20000000       -0.02000000
-------------------------------------------------------------------
 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 figures have been obtained by directly applying the VMD script from the calculation. The lines defining the cube edges have also been highlighted when appropriate.

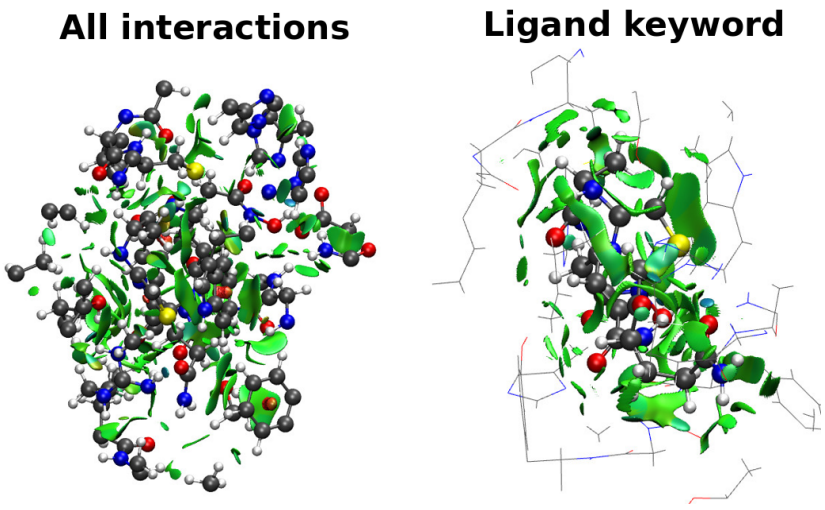

Figure 5: NCI analysis of the 2v5x-ligand interaction. Comparison of the isosurfaces obtained without the `LIGAND`(left) keyword and with it (right). 0.3 RDG isosurface. Colour code: -0.07(blue), 0.00(green), 0.07(red)

Choosing the interactions

The uracil dimer is a small system where several non-covalent interactions are at play: hydrogen bonds, van der Waals interactions and steric clashes. To reveal the details of these interactions, we can take advantage of the new calculation features:

```
2
uracil_1.xyz
uracil_2.xyz
FINE
OUTPUT 3
INTEGRATE
INTERMOLECULAR
CLUSTERING
RANGE 3
-0.2 -0.02
-0.02 0.02
0.02 0.2
ONAME uracil_dimer
```

Use of the CLUSTERING keyword separates the individual spatially distinct contributions of the NCI region based on underlying bond critical points. It also calculates the integration of each of the regions in ranges:

```
#-------------------------------------------------------------------------
                              NCICLUSTER
-------------------------------------------------------------------------
```

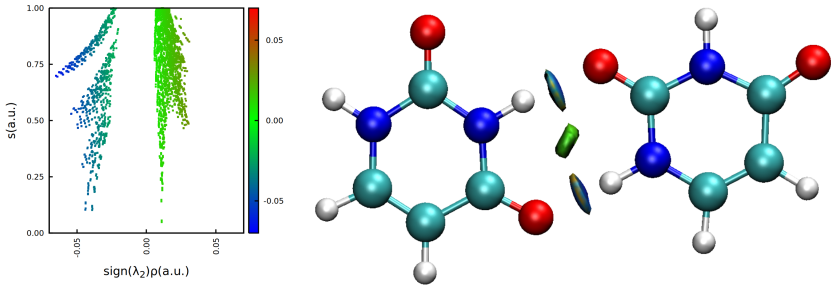

Figure 6: NCI analysis of the uracil dimer. (Left) RDG *vs* $sign(\lambda_2)\rho$ plot. (Right) 0.5 RDG isosurface. Colour code: -0.07(blue), 0.00(green), 0.07(red)

```
 Start -- Fri Jul 18 15:24:01 2025

 Gradient threshold:  0.386
 Number of critical points found:  3

-------------------------------------------------------------------------
      RANGE CLUSTERED INTEGRATION DATA over the volumes of rho^n
-------------------------------------------------------------------------
 Cluster 0
-------------------------------------------------------------------------
 Interval        :       -0.20000000       -0.02000000
-------------------------------------------------------------------------
 n=1.0           :        0.16812674
 n=1.5           :        0.03455973
 n=2.0           :        0.00728219
 n=2.5           :        0.00157460
 n=3.0           :        0.00034965
 n=4/3           :        0.05840127
 n=5/3           :        0.02050758
 Volume          :        4.26497364
```

The individual clusters are saved as separate .cube files, and a divided.vmd script could be used to visualise them.

If the NCIENERGY keyword is triggered, the calculation of energies with the equations (according to https://hal.science/hal-04943402v1/) also proceeds. Do note, this requires reading of the nci output file specifically called nci_ONAME.out file back into the code, and the software assume it to be the name, otherwise, it will give an error. The output of the calculation is:

```
-------------------------------------------------------------------------
                            NCIENERGY
-------------------------------------------------------------------------
 Calculating energy using the promolecular equation
 If your system contains sigma hole interactions,
```

```
 consider using the clustering mode for better energy accuracy
-----------------------------------------------------------------------
 NCI energies / kJ/mol
 E_sum   :        -53.12710583
 E_polar :        -49.39910501
 E_vdw   :        -3.72800083
-----------------------------------------------------------------------
```

Useful scripts

Using the VMD script

The program generates a script for visualisation 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 an RDG cut-off as specified by the keyword `RDG_CUTOFF` (otherwise, a default is used).

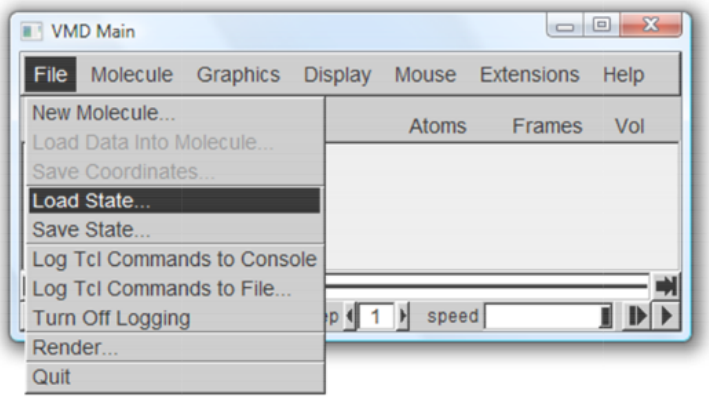

Figure 7: Image caption of the VMD dashboard.

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 the density cut-off

In order to generate figures ready of publication quality, the background needs to be coloured in white. This can be done by going to the GRAPHICS slash and selecting 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 NCIcolourr 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 colour 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 colour 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 ''
```