NCIRange

User Manual

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1 Introduction

Technological and scientific applications of supramolecular chemistry require a correct analysis of noncovalent interactions (NCI). The knowledge of the origin of the van der Waals forces, steric repulsion and hydrogen bonds into molecular association processes has allowed the control on self-assemblies. From this point, it has been possible to explain several natural processes involving protein, lipids and nucleic acids[1]. Likewise, it can be the source of inspiration in the design and tuning of molecular switches, electronics, and polymers[2, 3].

Several electron-density-based techniques have contributed to analyze, visualize, and interpret the NCI, e.g electron localisation function (ELF) and atoms in molecule theory (AIM). The study of the reduced density gradient, $s(\mathbf{r})$, has recently become popular to intuitively detect the NCI as an isosurface in the interacting region[4, 5].

The NCI isosurfaces are generated by a program called NCIPlot[6]. It takes a wavefunction file (.wfn), calculates its $s(\mathbf{r})$ and generates the following files: (1) Gaussian cube file (.cube) with density ($\rho(\mathbf{r})$; (2) Gaussian cube file (.cube) with $s(\mathbf{r})$; and (3) Visual Molecular Dynamics script (.vmd). With the VMD script and the Visual Molecular Dynamics Software NCI isosurfaces can be plotted.

Sometimes, a separated picture of the isosurfaces is necessary. The attractive or repulsive forces, likewise hydrogen bonds, can be conveniently visualized isolated from the rest. NCIRange solves this problem. This script takes the cube files

produced by NCIPlot and extracts the reduced density gradients regions. A new reduced density gradients cube file is generated, and optionally, a VMD script.

2   Installation

NCIRange is a Perl script, and therefore its main software requirement is a Perl interpreter. In all of Unix-type operating systems (**UOS**) is already available by default. In Windows operating systems (**WOS**), there are two popular distributions: (1) Active State and (2) Strawberry Perl. The NCIRange script, and additional files, can be requested to the author by writing an email to nestorcubillan@mail.uniatlantico.edu.co.

The installation in **UOS** is straightforward. A global installation is carried out by root user as:

```
mypc@root:~$ chmod ugo+x ncirange.pl
mypc@root:~$ cp ncirange.pl /usr/local/bin
```

Alternatively, it is possible to install the script on the HOME user:

```
mypc@myuser:~$ mkdir bin
mypc@myuser:~$ chmod u+x ncirange.pl
mypc@myuser:~$ cp ncirange bin/
mypc@myuser:~$ vi .bashrc
```

Then, add the line

```
export PATH = $PATH:/home/myuser/bin
```

Save and run the command:

```
mypc@myuser:~$ source .bashrc
```

On **WOS**:

```
C:\Users\myuser> perl -le "print $^X"
```

Copy the output (e.g. `C:\perl\bin\perl.exe})`,and run the following commands from the command prompt:

```
C:\Users\myuser> assoc .pl=PerlScript
C:\Users\myuser> ftype PerlScript=C:\perl\bin\perl.exe "%1" %*
```

Here, the folder containing the script can be moved to "`C:\Program files`" or another location and added to your PATH.

3   Usage

NCIRange is a command-line driven script. Its generic format is:

```
ncirange.pl -prefix XXX -range AA,BB:CC,DD -sign -vmd
```

The arguments you can pass to it are:

-prefix or -p	Prefix to cube files. eg. XXX-grad.cube and XXX-dens.cube
-range or -r	Range in ascendant order (AA<BB and CC<DD). Several ranges should be separated by colon (:)
-sign or -s	(OPTIONAL) The RDG values are extracted with the sign and value of the density
-vmd or -v	(OPTIONAL) Generate VMD file to plot RDG range
-help or -h	Print Help and exit
-version or -V	Print version information and exit

The script generates a new file with RDG values in the given range. The name of the output file is XXX-rang.cube. If -vmd option is chosen a file XXX-rang.vmd is created.

4   Examples

All capabilities of this script are shown with an example of hydrogen bonding of 1-(Methylamino)-1-ethanone with a water monomer (See Fig. 1). The results of NCIPlot calculations generate the Fig. 2. All surfaces were plotted with VMD software, and the colormaps were generated with the ncicolormap.gnu script and GNUPlot.
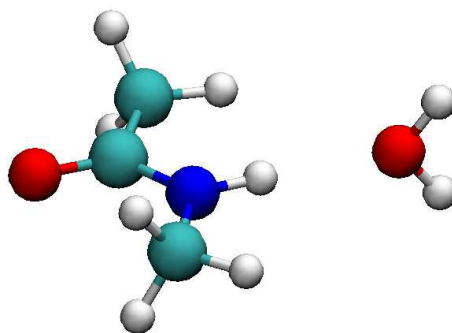

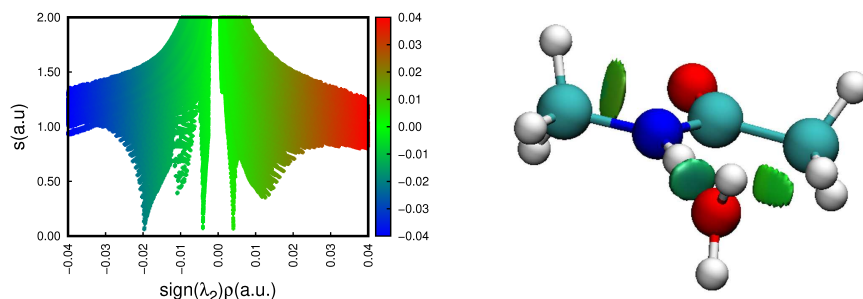Figure 1: Model of complex of 1-(Methylamino)-1-ethanone with a water monomer.

Figure 2: NCIColormap and NCIPlot of model showing all interactions

The first two examples show RDG values extracted using NCIRange that are associated to unsigned densities. In these cases, the extracted RDG value is associated to the absolute value of ρ. In the Fig. 3, the densities between 0.001 and 0.005 (van der Waals interactions), and 0.005 and 0.015.

```
ncirange.pl -p prueba -r 0.001,0.005 -v
ncirange.pl -p prueba -r 0.005,0.015 -v
```

It also is possible to extract RDG values associated to signed values of density. In the example, the attractive forces ($\rho < 0$) are shown — see Fig. 4. The
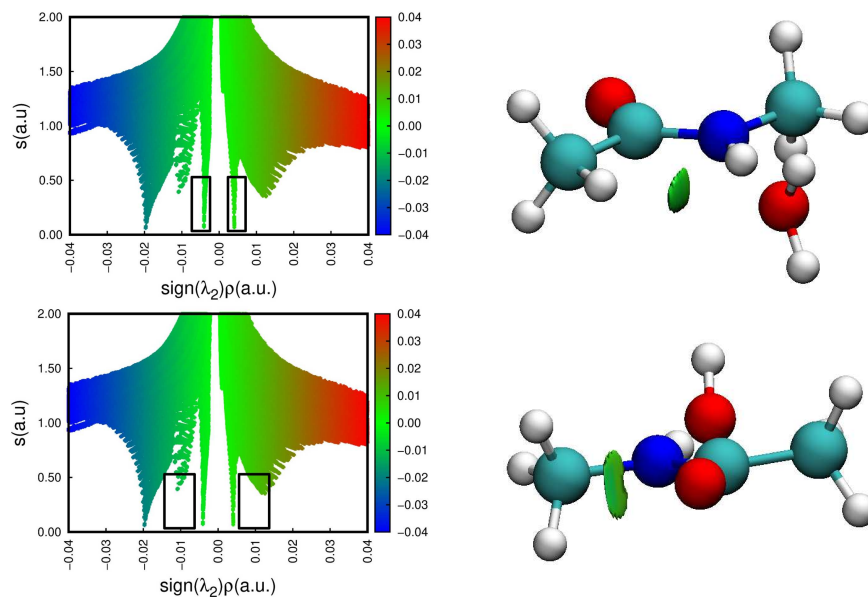

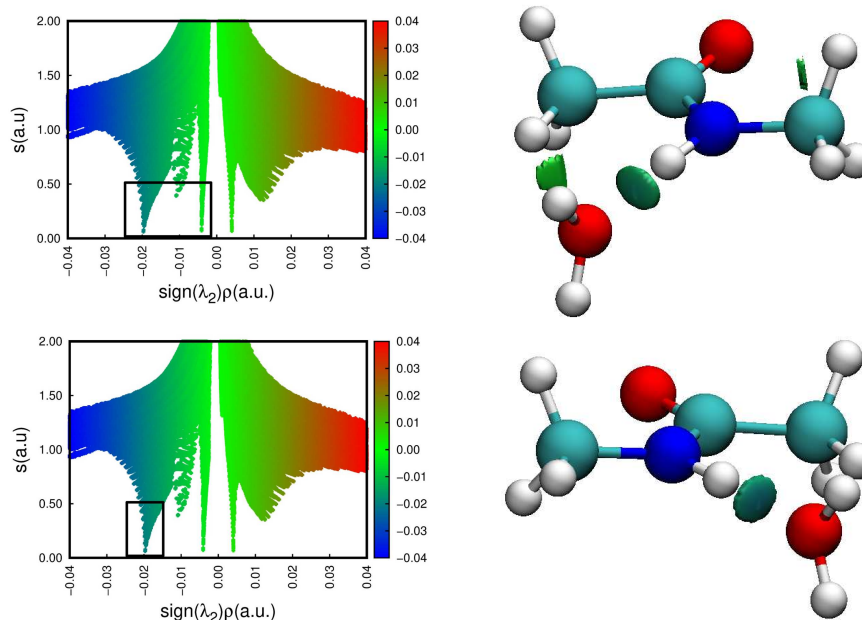Figure 3: NCIColormap and NCIPlot model showing RDG with absolute value of density

Figure 4: NCIColormap and NCIPlot of model extracting signed values of density

next graphs pair isolates the hydrogen bonding interaction, i.e. the region with ρ between -0.015 and -0.025.

```
ncirange.pl -p prueba -s -r -0.025,-0.001 -v
ncirange.pl -p prueba -s -r -0.025,-0.015 -v
```

The following example shows NCIRange extracting multiple ranges and signed values of density. In this case, the water-amine hydrogen bond and the attractive van der Waals interactions are shown — see Fig. 5.

```
ncirange.pl -p prueba -s -r -0.005,-0.001:-0.025,-0.015 -v
```
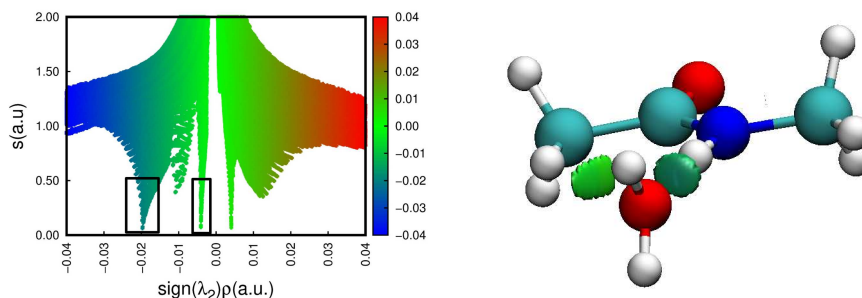

Figure 5: NCIColormap and NCIPlot of model

References

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[6] J. Contreras-García, E. R. Johnson, S. Keinan, R. Chaudret, J.-P. Piquemal, D. N. Beratan, and W. Yang, "NCIPLOT: A program for plotting noncovalent interaction regions," *J. Chem. Theory Comput.*, vol. 7, no. 3, pp. 625–632, 2011.

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