1. Get the wfn files

➢ *With a Gaussian03 output file from an IRC calculation*

- Read the output file (irc.out): read_irc irc.out
- Input: start number:
    - 0 to read the whole path
    - 1/-1 to read only from the reactant to the transition state/ transition state to the production (respectively)
    - TS number: structure number associated with the transition state
    - E min: minimum energy on the path

Two files are then obtained:
geom._α.inp *(α = tot, rev or fwd depending on the "start_number" selected); this is a Gaussian input containing the geometries of the different IRC structures and the Gaussian commands to obtain the wfn files for each point.*
irc_α.dat *(α = tot, rev or fwd depending on the "start_number" selected); dat file (can be read with gnuplot) containing the relative energy for each point of the path.*

- Submit geom._XXX.inp

The geom_XXX.wfn files (XXX = point number, XXX starts with 001) are obtained in output.

➢ *With a Gaussian09 output file from a dynamic calculation*

- Read the output file from BOMD dynamic (dyna.out): read_dyna dyna.out
- Input the number of points of the dynamic (npts)

The file geom._tot.inp is obtained: Gaussian input file that contains the geometries of the points of the dynamic and the Gaussian commands to obtain the wfn files for each point.

- Submit geom_tot.inp

The geom._XXX.wfn files are obtained in output

2. Get the NCI files

- Launch make_scan_nci.sh : *the files geomXXX-dens.cube,geomXXX-grad.cube and geomXXX.dat are obtained in output.*
- Launch scan_topo.sh: *the files geomXXX.wfn_topo.xyz (NCI Interaction Critical Points), geomXXX.wfn_topo.dat are obtained in output.*

3. Get the ELF files

- Launch xyz.sh: *the files *.sbf and geomXXX_elf.cube, geomXXX_esyn.cube and geomXXX_ebas.xyz are obtained in output.*
- Launch make_scan_elf.sh: *the files geom.XXX.wfn_pop.out, geomXXX.wfn_sumelf.out are obtained in output.*

ATTENTION: the different files used to launch the calculations can be modified in order to change the type of calculation done.

Program	Associated Input file
make_scan_nci.sh	nci.inp
scan_topo.sh	topo.inp
xyz.sh	grid.inp elf.inp rho.inp ebas_sbf.inp esbf.inp ysbf.inp exyz.inp
make_scan_elf.sh	grid.inp elf.inp rho.inp pop.inp

4. Get the animations

- Open one structure with vmd, coose the view point desired and save the state.
- Launch elf_nci_visualization.pl: "./elf_nci_visualization.pl input output_vmd_surface output_vmd_attractor"
- An example of input file is proposed in example-input-vnd-file. You must input
    - The number of the first and last geometry (starting from 1)
    - The type of picture you want (ELF, NCI or BOTH)
    - The vmd representation (CPK, licorice or line)
    - The ELF isosurface cutoff (if input=0, then default 0.8 value is used)
    - The NCI isosurface cutoff, color scale range (default 0.2, -5.0, 5.0)

Note: If BOTH keyword is specified then ELF comes before NCI)

- View point from the vmd previously saved

This will create the vmd files: output_vmd_surface output_vmd_attractor files

a. Obtaining a film and pictures of the evolution of the surfaces

- Open vmd and load output_vmd_surface state: *tga format pictures are obtained for every point.*
- Launch tga2gifanim: *a gif animation named aro_anim.gif and gif pictures for every previous tga file are obtained*

b. Obtaining a film and pictures of the evolution of ELF attractors and NCI ICPs

- Open vmd and load output_vmd_attractor *tga format pictures are obtained for every point.*
- Launch tga2gifanim: *a gif animation named aro_anim.gif and gif pictures for every previous tga file are obtained*

c. Obtaining a film and pictures of the evolution of the 2D NCI graph

- Launch gnup.sh: *png files for each geomXXX.dat file are obtained*
- Launch png2gifanim: *a gif animation named aro_anim.gif and gif pictures for every previous png file are obtained*