Using TopMod for ELF

http://www.lct.jussieu.fr/pagesperso/silvi/manual/manual.html

Run top_grid then top_bas (twice: once for ELF then for rho) then top_pop.

User input in yellow, ... indicates program output.

./top_grid

input .wfn file

ethene.wfn

.....

output density? (y/n)

y

.....

input the origin of the grid x,y,z

-5 -7 -7

input edges along x,y,z

10 14 14

input the number of intervals along x,y,z

100 140 140

"In output the program generates title_elf.sbf (and title_rho.sbf if requested files) file(s) in which title is the first non-blank characters of the title in gaussian input" (wfn file).

./top_bas

function: elf/rho

elf

input .wfn file

ethene.wfn

.....

accuracy: 0 very high, 1 high, 2 medium

1 (1 is recommended in manual. Any times I've used 2 I got the same answers as 1 but I haven't tested it properly to see if that is always the case or whether there are significant time savings by using 2.)

find external core shell attractors?

n (If n it merges the external core shell basins, if y you get the core shell basins all located close to the nuclei – not usually needed for the types of systems we are considering.)

[There is apparently an option here for atoms with pseudo potentials (choose 1 for large core or 2 for small core for each atom with a PP). However, the G03 .wfn files don't include output from PPs so I don't know how you would ever get this option – it hasn't ever appeared for me]

.....

search mode: 0 automatic, >0 number of attractors in input, <0 fast

0 (<0: fast automatic from the current grid, finds only attractors within the box; 0: full automatic, search in the whole molecular space) Any times I've used -1 I got the same answers as 0 but I haven't tested it properly to see if that is always the case or whether there are significant time savings by using -1.) See manual for other options (>0 poss but extra input required – I have never tried it.)

.....

assign grid points?

y

"In output the program writes one file: title_ebas.sbf or title_ras.sbf" (according to the chosen function elf/rho) "to be used by top_pop and one input file for top_bas named temp.bas."

(I don't really understand the next paragraph (from the manual): "The temp.bas file corresponds to the input attractor mode, it can be generated with a different wave function (for example with a smaller basis set) which nevertheless yields the same overall topology and without grid point assignment. In this case it is not necessary to run top_grid before. This procedure is recommended for large systems. Do not forget to update the wfn file name in temp.bas if another wfn file is used.")

.....

./top_bas

function: elf/rho

rho (not sure if it is necessary to run for rho also but it is much quicker than the elf step anyway)

input .wfn file

ethene.wfn

.....

accuracy: 0 very high, 1 high, 2 medium

1

.....

assign grid points?

y

.....

./top_pop (usually need to pipe output for large molecules)

input .wfn file

ethene.wfn

.....

threshold for integration tol ==> 10-tol

7 (integration threshold (recommended value 7) – I have never tried anything else and have no idea what it actually means)

number of ELF and AIM basins considered

0 0 numbers of ELF and AIM basins considered (if 0 all the basins are taken into account in the calculation)

Steps 4 and 5 are skipped if the above input is 0 0. I have never tried anything other than 0 0 so I don't know how it works.

Example output for ethene.

[rzepa@login-0 top2]$ ./top_grid

input .wfn file

ethene.wfn

8 molecular orbitals

72 primitive functions

6 atomic centres

fmt: read unexpected character

apparent state: unit 1 named ethene.wfn

last format: (a4,20x,3f12.8,10x,f6.2)

lately reading sequential formatted external IO

Aborted

[rzepa@login-0 top2]$ dos2unix ethene.wfn

```
dos2unix: converting file ethene.wfn to UNIX format ...
[rzepa@login-0 top2]$ ./top_grid
  input .wfn file
ethene.wfn
   8 molecular orbitals
  72 primitive functions
   6 atomic centres
      2628 non zero density matrix elements among       2628
  output density? (y/n)
y
  indicative origin of the grid
      -5.000000   -6.745468   -7.342413
  indicative edges along x,y,z
      10.000000   13.490936   14.684825
  input the origin of the grid x,y,z
-5 -7 -7
  input edges along x,y,z
10 14 14
  input the number of intervals along x,y,z
100 140 140
 101 grid points along x axis
 141 grid points along y axis
 141 grid points along z axis
   elapsed time     24.14sec

  2007981 elf values have been written on file: ethene_elf.sbf
  2007981 values of the density have been written on file:ethene_rho.sbf
STOP normal termination  statement executed
[rzepa@login-0 top2]$ ./top_bas
  function: elf/rho
elf
  input .wfn file
ethene.wfn
```

```
  8 molecular orbitals
 72 primitive functions
  6 atomic centres
     2628 non zero density matrix elements among      2628
 accuracy: 0 very high, 1 high, 2 medium
1
 find external core shell attractors?
n

 Core basins

atom                attractor position     ELF       eigenvalues        radius

C1                0.000   0.000   1.258   1.000  -0.003  -0.003  -0.003
                0.000  -0.476   1.553   0.086                    0.560
C2                0.000   0.000  -1.257   1.000  -0.003  -0.003  -0.003 0.560


 search mode: 0 automatic, >0 number of attractors in input, <0 fast
0

  elapsed time in attractor search     0.33 sec.


 8 attractors found
 assign grid points?
y


  origin          -5.0000     -7.0000     -7.0000
  edge            10.0000     14.0000     14.0000
  step            0.1000      0.1000      0.1000
  grid points          100         140         140
```

total number of grid points: 2007981

elapsed time in sort procedure 1.30 sec.
elapsed time in init step 1.99 sec.
considered grid points 881341
10% done 1.08 s. spent 10.80 s. expected
20% done 7.89 s. spent 39.45 s. expected
30% done 25.28 s. spent 84.27 s. expected
40% done 30.59 s. spent 76.48 s. expected
50% done 35.72 s. spent 71.44 s. expected
60% done 41.45 s. spent 69.08 s. expected
70% done 48.33 s. spent 69.04 s. expected
80% done 54.85 s. spent 68.56 s. expected
90% done 60.26 s. spent 66.96 s. expected
100% done 65.66 s. spent 65.66 s. expected

elapsed time in search step 67.65 sec.
number of attractors: 8
border points: 26682 3047

elapsed time in attractor assignment 0.07 sec.

1	0.000	0.000	1.258	1.000	C(C1)	814	814	0.81	5
2	0.000	0.000	-1.257	1.000	C(C2)	814	814	0.81	5
3	0.000	1.837	2.389	1.000	V(H1,C1)	172904	89690	89.69	2
4	0.000	-1.837	2.389	1.000	V(H2,C1)	171848	88664	88.66	2

5	0.000	-1.837	-2.389	1.000	V(H3,C2)	171719	88605	88.61	2
6	0.000	1.837	-2.389	1.000	V(H4,C2)	172930	89745	89.75	2
7	0.666	0.000	0.000	0.937	V(C1,C2)	94863	55603	55.60	3
8	-0.666	0.000	0.000	0.937	V(C1,C2)	95449	56124	56.12	3

unassigned grid points 1126640 0

distances from nuclei (A)

V(H1,C1) C1
1.142
V(H2,C1) C1
1.142
V(H3,C2) C2
1.142
V(H4,C2) C2
1.142
V(C1,C2) C1 C2
0.753 0.753
V(C1,C2) C1 C2
0.753 0.753

angles around core attractors

V(H1,C1)	C(C1)	V(H2,C1)	116.733
V(H1,C1)	C(C1)	V(C1,C2)	117.616
V(H1,C1)	C(C1)	V(C1,C2)	117.616
V(H2,C1)	C(C1)	V(C1,C2)	117.616
V(H2,C1)	C(C1)	V(C1,C2)	117.616
V(C1,C2)	C(C1)	V(C1,C2)	55.791
V(H3,C2)	C(C2)	V(H4,C2)	116.727
V(H3,C2)	C(C2)	V(C1,C2)	117.618

```
V(H3,C2)       C(C2)          V(C1,C2)          117.618
V(H4,C2)       C(C2)          V(C1,C2)          117.618
V(H4,C2)       C(C2)          V(C1,C2)          117.618
V(C1,C2)       C(C2)          V(C1,C2)           55.796

 angles around polysynaptic attractors

C1  V(C1,C2)       C2       124.207
C1  V(C1,C2)       C2       124.207
[rzepa@login-0 top2]$ ./top_bas
  function: elf/rho
rho
  input .wfn file
ethene.wfn
   8 molecular orbitals
  72 primitive functions
   6 atomic centres
     2628 non zero density matrix elements among      2628
  accuracy: 0 very high, 1 high, 2 medium
1
Atom(C1  )        0.000   0.000   1.257
Atom(H1  )        0.000   1.716   2.324
Atom(H2  )        0.000  -1.716   2.324
Atom(C2  )        0.000   0.000  -1.257
Atom(H3  )        0.000  -1.716  -2.324
Atom(H4  )        0.000   1.716  -2.324


 assign grid points?
y


  origin          -5.0000     -7.0000     -7.0000
```

edge 10.0000 14.0000 14.0000
step 0.1000 0.1000 0.1000
grid points 100 140 140

total number of grid points: 2007981

elapsed time in sort procedure 1.13 sec.
elapsed time in init step 1.38 sec.
considered grid points 705841
10% done 3.94 s. spent 39.40 s. expected
20% done 10.56 s. spent 52.80 s. expected
30% done 17.60 s. spent 58.67 s. expected
40% done 23.58 s. spent 58.95 s. expected
50% done 29.47 s. spent 58.94 s. expected
60% done 34.56 s. spent 57.60 s. expected
70% done 39.43 s. spent 56.33 s. expected
80% done 44.26 s. spent 55.33 s. expected
90% done 49.15 s. spent 54.61 s. expected
100% done 54.05 s. spent 54.05 s. expected

elapsed time in search step 55.43 sec.
number of attractors: 6
border points: 31675 4404

1	0.000	0.000	1.257	0.000	Atom(C1)	158095	158095	158.09	5
2	0.000	1.716	2.324	0.000	Atom(H1)	96561	96561	96.56	5
3	0.000	-1.716	2.324	0.000	Atom(H2)	96578	96578	96.58	5
4	0.000	0.000	-1.257	0.000	Atom(C2)	161423	161423	161.42	5

```
  5   0.000  -1.716  -2.324   0.000  Atom(H3  )       96599  96599   96.60  5
  6   0.000   1.716  -2.324   0.000  Atom(H4  )       96585  96585   96.59  5


 unassigned grid points   1302140         0
[rzepa@login-0 top2]$ ./top_pop
 input .wfn file
ethene.wfn
  8 molecular orbitals
 72 primitive functions
  6 atomic centres
 threshold for integration tol ==> 10-tol
7
 number of ELF and AIM basins considered
0 0
 ethene_ebas.sbf
   number of localization basins    8
 ethene_rbas.sbf
   number of atomic basins    6
   total integrated density    15.999464
   total fluctuation     0.000536


 basin             vol.    pop.    pab     paa     pbb     sigma2  lambda


 1 C(C1)           0.81    2.09    1.09    0.18    0.18    0.26    0.12
 2 C(C2)           0.81    2.09    1.09    0.18    0.18    0.26    0.12
 3 V(H1,C1)       89.69    2.10    1.11    0.37    0.37    0.63    0.30
 4 V(H2,C1)       88.66    2.06    1.06    0.34    0.34    0.62    0.30
 5 V(H3,C2)       88.61    2.05    1.05    0.34    0.34    0.62    0.30
 6 V(H4,C2)       89.75    2.10    1.11    0.37    0.37    0.63    0.30
 7 V(C1,C2)       55.60    1.70    0.72    0.34    0.34    0.94    0.56
```

8 V(C1,C2)	56.12	1.80	0.81	0.40	0.40	0.98	0.54

sum of populations 15.994332

orbital contributions

	1	2	3	4	5	6	7	8
C(C1)	0.95	0.95	0.03	0.03	0.03	0.04	0.02	0.04
C(C2)	0.95	0.95	0.03	0.03	0.03	0.04	0.02	0.04
V(H1,C1)	0.02	0.02	0.23	0.46	0.41	0.31	0.47	0.19
V(H2,C1)	0.01	0.01	0.23	0.45	0.41	0.30	0.47	0.18
V(H3,C2)	0.01	0.01	0.23	0.45	0.41	0.30	0.47	0.18
V(H4,C2)	0.02	0.02	0.23	0.46	0.41	0.31	0.47	0.19
V(C1,C2)	0.02	0.02	0.48	0.06	0.15	0.33	0.04	0.59
V(C1,C2)	0.02	0.02	0.52	0.06	0.16	0.37	0.04	0.59

atomic contributions

	C1	H1	H2	C2	H3	H4
C(C1)	2.09	0.00	0.00	0.00	0.00	0.00
C(C2)	0.00	0.00	0.00	2.09	0.00	0.00

V(H1,C1)	1.17	0.93	0.00	0.00	0.00	0.00
V(H2,C1)	1.13	0.00	0.93	0.00	0.00	0.00
V(H3,C2)	0.00	0.00	0.00	1.13	0.93	0.00
V(H4,C2)	0.00	0.00	0.00	1.18	0.00	0.93
V(C1,C2)	0.86	0.00	0.00	0.84	0.00	0.00
V(C1,C2)	0.91	0.00	0.00	0.89	0.00	0.00

alpha entropy 0.041871

beta entropy 0.041871

total entropy 0.007612

cross exchange contributions (covariance)

	1	2	3	4	5	6	7	8
C(C1)	1.83	0.00	0.07	0.07	0.01	0.01	0.05	0.05
C(C2)	0.00	1.83	0.01	0.01	0.07	0.07	0.05	0.05
V(H1,C1)	0.07	0.01	1.47	0.19	0.03	0.03	0.15	0.15
V(H2,C1)	0.07	0.01	0.19	1.44	0.03	0.03	0.14	0.15
V(H3,C2)	0.01	0.07	0.03	0.03	1.43	0.19	0.14	0.15
V(H4,C2)	0.01	0.07	0.03	0.03	0.19	1.47	0.15	0.15
V(C1,C2)	0.05	0.05	0.15	0.14	0.14	0.15	0.75	0.26
V(C1,C2)	0.05	0.05	0.15	0.15	0.15	0.15	0.26	0.82

elapsed time 4.85sec.

AIM ANALYSIS

basin	vol.	pop.	pab	paa	pbb	sigma2	lambda
Atom(C1)	158.09	6.17	9.51	7.42	7.42	1.99	0.32
Atom(H1)	96.56	0.93	0.21	0.02	0.02	0.53	0.57
Atom(H2)	96.58	0.93	0.21	0.02	0.02	0.53	0.57
Atom(C2)	161.42	6.12	9.35	7.28	7.28	1.99	0.32
Atom(H3)	96.60	0.93	0.21	0.02	0.02	0.53	0.57
Atom(H4)	96.59	0.93	0.21	0.02	0.02	0.53	0.57

sum of atomic populations 15.983784

orbital contributions

	1	2	3	4	5	6	7	8
Atom(C1)	1.00	1.00	0.87	0.62	0.58	0.73	0.41	0.97
Atom(H1)	0.00	0.00	0.07	0.19	0.21	0.14	0.30	0.02
Atom(H2)	0.00	0.00	0.07	0.19	0.21	0.14	0.30	0.02
Atom(C2)	1.00	1.00	0.85	0.62	0.57	0.71	0.41	0.96

Atom(H3) 0.00 0.00 0.07 0.19 0.21 0.14 0.30 0.02
Atom(H4) 0.00 0.00 0.07 0.19 0.21 0.14 0.30 0.02

alpha entropy 0.014286

beta entropy 0.014286

total entropy 0.002498

cross exchange contributions (covariance)

1 2 3 4 5 6

Atom(C1) 4.18 0.48 0.48 0.98 0.03 0.03
Atom(H1) 0.48 0.40 0.01 0.03 0.01 0.00
Atom(H2) 0.48 0.01 0.40 0.03 0.00 0.01
Atom(C2) 0.98 0.03 0.03 4.13 0.48 0.48
Atom(H3) 0.03 0.01 0.00 0.48 0.40 0.01
Atom(H4) 0.03 0.00 0.01 0.48 0.01 0.40

elapsed time 4.85sec.
[rzepa@login-0 top2]$