Supporting Informations
for
A Program Package for the Calculation of Origin Independent Electron Current Density and Derived Magnetic Properties in Molecular Systems

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1 Introduction

SYSMOIC is a program package for the calculation and visualization of the magnetically induced, origin independent electron current density, by means of the continuous transformation of the origin of the current density (CTOCD) method, for closed-shell molecular systems at the Density Function Theory (DFT) level of approximation as well as at the Hartree-Fock (HF) level.

More precisely, the package provides methods for the calculation of the quantum mechanical, second-rank electron current density tensor, which is used to calculate the first-order current density vector (CDT), for any orientation of an inducing external magnetic field, a number of related density properties, the vorticity tensor (VT) and anisotropies of both CDT and VT.

1.1 Version

Current package version: **SYSMOIC - 1.1**.

As a result of maintenance, new versions of the package will be released. The first digit will be incremented in case of a major revision, due to updating core libraries and/or addition of new functionalities; the second digit will be incremented in case of minor

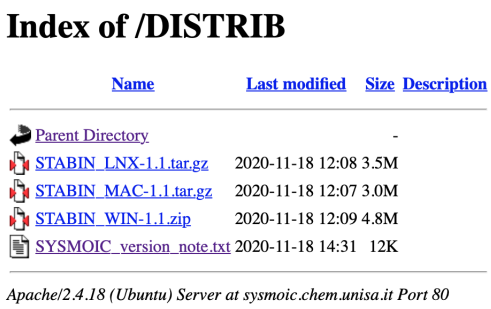
revisions. Users are kindly requested to visit periodically both manual and distribution to check for new versions of the package.

The full set of worked examples, reported in this manual and in the reference paper, can be downloaded here.

For queries or to report any bug, please e-mail to authors. Please, e-mail to authors also to inform them in case of package download (not mandatory, to be informed of new releases).

2 Installation

Open your preferred browser and type the address `http://SYSMOIC.chem.unisa.it/DISTRIB`, alternatively click here. Something like that should appear



Index of /DISTRIB

Name	Last modified	Size	Description
Parent Directory		-	
STABIN_LNX-1.1.tar.gz	2020-11-18 12:08	3.5M	
STABIN_MAC-1.1.tar.gz	2020-11-18 12:07	3.0M	
STABIN_WIN-1.1.zip	2020-11-18 12:09	4.8M	
SYSMOIC_version_note.txt	2020-11-18 14:31	12K	

Apache/2.4.18 (Ubuntu) Server at sysmoic.chem.unisa.it Port 80

`SYSMOIC_version_note.txt` reports news on revisions made with respect to the previous version of the package.

To download stand-alone executable programs of the package click on

- `STABIN_LNX-1.1.tar.gz` for Linux systems
- `STABIN_MAC-1.1.tar.gz` for Mac
- `STABIN_WIN-1.1.zip` for Windows

For both Linux and Mac systems, close the browser and open a terminal; change directory to the folder were the installation file has been downloaded and type the following command

```
prompt> tar -zxf STABIN_XXX-1.1.tar.gz
```

A folder `STABIN` is generated containing the SYSMOIC executable files, which can be copied in `/usr/local/bin/`, or the folder itself moved to, let say, `/usr/local/SYSMOIC/`. In the latter case, the `PATH` environmental variable must be updated to run executable in `/user/local/SYSMOIC/STABIN`.

For Windows systems, go to the folder where `STABIN_WIN-1.1.zip` has been downloaded and extract it. A new folder named `STABIN` should be generated containing the stand-alone Windows executables. Move the `STABIN` folder where you prefer and adjust the

PATH environment variable in order to execute the package programs from any terminal prompt.

SYSMOIC executable programs have been compiled to run standalone, apart the v3d program which requires OpenGL. Usually OpenGL is already installed on Ubuntu and other Linux systems, otherwise it can be installed through the apt-get install command.

3 How to use

Three different routes for the calculation of the magnetically induced current density are presented here in the following. Examples are provided for benzene, borazine and planar cyclooctatetraene.

- Route-1, old-fashion SYSMO calculation, which can only be at the HF level of theory, with maximum basis function type f;
- Route-2 mixed Gaussian-SYSMO, which can be done at both the HF and DFT, with maximum basis function type f;
- Route-3, Gaussian calculation, HF or DFT, with maximum basis function type m.

After each type of calculation, first-order perturbed wavefunctions will be ready for the subsequent current density determinations by means of the IC (Induced Current) programs.

3.1 Route-1

Preparing SYSMO input files is fairly simple. First of all, one has to consider that SYSMO programs must be used in some sequence depending on which kind of results are wanted. Then, each SYSMO programs has its own separate input. Within the distribution there is a utility to help preparing the SYSMO input file. The name of the utility is MOMO and can be used on the command line as

```
prompt> MOMO some_file.ext
```

where 'ext' can be one of the following:

xyz in this case some_file must contain a free-format list of Cartesian coordinates in atomic units, one atom per line beginning with the chemical symbol followed by the x, y, z values;

XYZ the same as for xyz with Cartesian coordinates in Angstrom;

fchk some_file is the formatted check point file from a Gaussian calculation (G09 and G16 are supported).

To try it, go to the benzene folder and type

```
prompt> MOMO benzene.fchk
```

the following should appear on the screen

```
*************
*  M O M O  *
*************
Version 07/03/2020-17:16,Covid-19,fase-I
BENZENE D6H GEO OPT B3LYP 6-31G*
RB3LYP
6-31G(D)
12  atoms plotted
12  bonds plotted
Clar.............(Clar)=  0.00
TRIANGULATION.....(tri)=  F
BOND ORDERS........(bo)=  F
SYMBOLS...........(sym)=  F
CARTESIAN AXIS....(ass)=  F
SLATER............(sla)=  F
HYDROGENS.........(hyd)=  T
GHOST ATOMS.......(gho)=  F
BALL SCALE........(sca)=  0.30
AROMA BONDS.......(aro)=******
SYMMETRY..........(spg)= C1
COMMAND SHELL.....(shl)= bash
CALCULATION TYPE..(cty)= CHF
ENTER 'com' FOR MORE COMMANDS
```

The `MOMO` program does many things, for the moment let us consider only the calculation type and symmetry. Calculation type can be changed typing

```
cty CHF
```

or

```
cty RPA
```

where `CHF` stands for Coupled Hartree-Fock and `RPA` for Random Phase Approximation, the default is `CHF`. To set the symmetry point group one has to type directly the name of the group in Schoenflies notation after the `spg` flag as

```
spg D6h
```

or just typing `spg` alone. This latter method works only if a gaussian `log` file is contained in the working folder with the same root-name of the `fchk` given above. Also the commad shell can be changed by typing `shl csh` or `shl bash`.
For a current density calculation the `cty` must be set to `CHF`. Then, let us assume the following setting

```
Clar.............(Clar)=  0.00
TRIANGULATION.....(tri)=  F
```

```
BOND ORDERS........(bo)=  F
SYMBOLS............(sym)=  F
CARTESIAN AXIS....(ass)=  F
SLATER.............(sla)=  F
HYDROGENS.........(hyd)=  T
GHOST ATOMS.......(gho)=  F
BALL SCALE........(sca)=  0.30
AROMA BONDS.......(aro)=******
SYMMETRY..........(spg)= D6H
COMMAND SHELL.....(shl)= bash
CALCULATION TYPE..(cty)= CHF
```

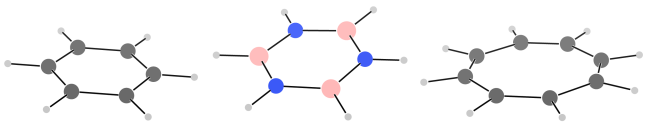
Typing the command

```
write benzene.isy
```

and confirming `y` to write or overwrite, a file `benzene.isy` (`isy` standing for input sysmo) will be generated containing a bash script to perform SYSMO calculation of dipole electric and magnetic properties at the Coupled Hartree-Fock Pertubation theory (CHFPT) approximation. To exit from the `MOMO` program type `q`. Rigth now, a new file `benzene.fchk.v3d` should be present in the folder. Its content can be visualized using the command 4.6

```
prompt> v3d benzene.fchk.v3d
```

a graphic window should appear with the molecular model (use mouse to rotate, translate and magnify as usual).



To set the calculation to perform only electric or magnetic properties, some editing must be done. The `benzene.isy` file should contain something like that:

```
 1 #!/bin/bash
 2 mo230xl << next
 3 BENZENE D6H GEO OPT B3LYP 6-31G*
 4
 5 D6H
 6 C1          0.00000000E+00    2.63892871E+00    0.00000000E+00
 7 S   6
 8 3.04752488E+03  1.83473713E-03
 9 4.57369518E+02  1.40373228E-02
10 1.03948685E+02  6.88426223E-02
11 2.92101553E+01  2.32184443E-01
12 9.28666296E+00  4.67941348E-01
13 3.16392696E+00  3.62311985E-01
```

```
14 S   3
15 7.86827235E+00 -1.19332420E-01
16 1.88128854E+00 -1.60854152E-01
17 5.44249258E-01  1.14345644E+00
18 P   3
19 7.86827235E+00  6.89990666E-02
20 1.88128854E+00  3.16423961E-01
21 5.44249258E-01  7.44308291E-01
22 S   1
23 1.68714478E-01  1.00000000E+00
24 P   1
25 1.68714478E-01  1.00000000E+00
26 D   1
27 8.00000000E-01  1.00000000E+00
28 C2  C1      2.28537930E+00    1.31946435E+00   -9.86076132E-32
29 C2  C1      2.28537930E+00   -1.31946435E+00    0.00000000E+00
30 C2  C1     -3.23175560E-16   -2.63892871E+00    2.31144182E-41
31 C2  C1     -2.28537930E+00   -1.31946435E+00    0.00000000E+00
32 C2  C1     -2.28537930E+00    1.31946435E+00    0.00000000E+00
33 H1          0.00000000E+00    4.69321902E+00    0.00000000E+00
34 S   3
35 1.87311370E+01  3.34946043E-02
36 2.82539436E+00  2.34726953E-01
37 6.40121692E-01  8.13757326E-01
38 S   1
39 1.61277759E-01  1.00000000E+00
40 H2  H1      4.06444689E+00    2.34660951E+00    0.00000000E+00
41 H2  H1      4.06444689E+00   -2.34660951E+00    0.00000000E+00
42 H2  H1     -5.74753565E-16   -4.69321902E+00    6.13364102E-41
43 H2  H1     -4.06444689E+00   -2.34660951E+00    0.00000000E+00
44 H2  H1     -4.06444689E+00    2.34660951E+00    0.00000000E+00
45
46 next
47 if [ $? == 0 ]; then
48 mo400xl << next
49 BENZENE D6H GEO OPT B3LYP 6-31G*
50 SODILI 1E-6 EOSCISTOP 50
51 gaumos benzene.fchk xyz
52
53 21
54 next
55 if [ $? == 0 ]; then
56 mo600xl << next
57 BENZENE D6H GEO OPT B3LYP 6-31G*
58
59 momento-di-dipolo salva
```

```
60 momento-lineare   salva
61 momento-angolare  salva
62
63 next
64 if [ $? == 0 ]; then
65 mo690xl << next
66 BENZENE D6H GEO OPT B3LYP 6-31G*
67 HFEXCHANGE x.xx
68
69
70 next
71 if [ $? == 0 ]; then
72 mo710xl << next
73 BENZENE D6H GEO OPT B3LYP 6-31G*
74 HFEXCHANGE 0.20
75
76
77 next
78 if [ $? == 0 ]; then
79 rm -f fort.4 fort.20
80 tar -a -cf benzene.tgz fort.*
81 rm -f fort.*
82 fi
83 fi
84 fi
85 fi
86 fi
87 exit
```

In order to have a script to perform only a magnetic perturbed calculation, lines from 64 to 70 must be deleted as well as line 82. Moreover, to force a calculation according to Route-1, lines 51 and 74 must be deleted too and the string `DIIS` must be added at the end of line 50. The `benzene.isy` file should now look as

```
1 #!/bin/bash
2 mo230xl << next
3 BENZENE D6H GEO OPT B3LYP 6-31G*
4
5 D6H
6 C1          0.00000000E+00    2.63892871E+00    0.00000000E+00
7 S   6
8 3.04752488E+03  1.83473713E-03
9 4.57369518E+02  1.40373228E-02
10 1.03948685E+02  6.88426223E-02
11 2.92101553E+01  2.32184443E-01
12 9.28666296E+00  4.67941348E-01
13 3.16392696E+00  3.62311985E-01
```

```
14 S   3
15 7.86827235E+00 -1.19332420E-01
16 1.88128854E+00 -1.60854152E-01
17 5.44249258E-01  1.14345644E+00
18 P   3
19 7.86827235E+00  6.89990666E-02
20 1.88128854E+00  3.16423961E-01
21 5.44249258E-01  7.44308291E-01
22 S   1
23 1.68714478E-01  1.00000000E+00
24 P   1
25 1.68714478E-01  1.00000000E+00
26 D   1
27 8.00000000E-01  1.00000000E+00
28 C2  C1      2.28537930E+00    1.31946435E+00   -9.86076132E-32
29 C2  C1      2.28537930E+00   -1.31946435E+00    0.00000000E+00
30 C2  C1     -3.23175560E-16   -2.63892871E+00    2.31144182E-41
31 C2  C1     -2.28537930E+00   -1.31946435E+00    0.00000000E+00
32 C2  C1     -2.28537930E+00    1.31946435E+00    0.00000000E+00
33 H1          0.00000000E+00    4.69321902E+00    0.00000000E+00
34 S   3
35 1.87311370E+01  3.34946043E-02
36 2.82539436E+00  2.34726953E-01
37 6.40121692E-01  8.13757326E-01
38 S   1
39 1.61277759E-01  1.00000000E+00
40 H2  H1      4.06444689E+00    2.34660951E+00    0.00000000E+00
41 H2  H1      4.06444689E+00   -2.34660951E+00    0.00000000E+00
42 H2  H1     -5.74753565E-16   -4.69321902E+00    6.13364102E-41
43 H2  H1     -4.06444689E+00   -2.34660951E+00    0.00000000E+00
44 H2  H1     -4.06444689E+00    2.34660951E+00    0.00000000E+00
45
46 next
47 if [ $? == 0 ]; then
48 mo400xl << next
49 BENZENE D6H GEO OPT B3LYP 6-31G*
50 SODILI 1E-6 EOSCISTOP 50 DIIS
51
52 21
53 next
54 if [ $? == 0 ]; then
55 mo600xl << next
56 BENZENE D6H GEO OPT B3LYP 6-31G*
57
58 momento-di-dipolo salva
59 momento-lineare   salva
```

```
60 momento-angolare  salva
61
62 next
63 if [ $? == 0 ]; then
64 mo710xl << next
65 BENZENE D6H GEO OPT B3LYP 6-31G*
66
67
68 next
69 if [ $? == 0 ]; then
70 rm -f fort.4 fort.20
71 tar -a -cf benzene.tgz fort.*
72 rm -f fort.*
73 fi
74 fi
75 fi
76 fi
77 exit
```

The script is ready and can be run using the command

```
prompt> ./benzene.isy >& benzene.osy &
```

After a while (or much more depending on the size of the actual molecule) the calculation is done and a couple of more files `benzene.osy` and `benzene.tgz` (or `benzene.fsy`, see here below for details) will appear in the current folder.

The `benzene.osy` file collects the output of the various SYSMO programs used by the script and it should be checked to see whether a string like `CONCLUSIONE NORMALE DI MO***XL` is present, one for each program.

The `benzene.tgz` is a tar-zipped file collecting some FORTRAN files, i.e., `fort.3, fort.11, fort.23`, and `fort.28`, which can be restored using the command

```
prompt> tar -zxf benzene.tgz
```

and deleted once used and no more needed. These files are required by the current density calculations 4.

A different way to pack together files `fort.3, fort.11, fort.23`, and `fort.28` is provided. In order to use this alternative, line 71 must be replaced with `pack benzene`, or `pack` *`file_name`* as desired. The `pack` command produces `benzene.fsy`, which can be unpacked using the command `unpack benzene`, any suffix is required. Windows users can use this commands instead of the Unix `tar` command.

Some concluding remarks for this section are as follows.

- The example above is for the benzene molecule, however nothing changes for other systems, apart from some attention to be payed on the permutation of the Cartesian coordinates. For example, for the borazine case one more command should be issued to `MOMO` to exchange x and y coordinates, typing the command `yxz` before writing the `borazine.isy` file.

- Geometry and basis set are read in from the `fchk` file, however this does not mean any strict dependence on the Gaussian package for Route-1. As mentioned, `MOMO` can read the Cartesian geometry from a different file with `xyz` or `XYZ` extensions, or even can be typed directly within the SYSMO input file. This latter way is convenient in symmetric cases, as the `mo230xl` program requires only symmetry unique atomic centers, the remaining are generated automatically.

- Basis set can be download from the web and copied within the `isy` file. A particularly reach basis set source can be found here.

- Depending on the size of the molecule under study, SYSMO programs of the extra large collection, i.e., those programs ending with an `xl`, can ask for more memory. In this case the amount of required memory can be modified on the running command (see lines 2, 48, 55, and 64) using `mo***xl -MEMR Nreal -MEMI Nint << next` , where `Nreal` and `Nint` are the number of `real*8` and `integer*4` kilo-words needed to run the calculation. An estimation of the actual amount of required memory is determined by the `MOMO` program, which writes the bash/csh script to perform the calculation with each `mo***xl -MEMR Nreal -MEMI Nint << next` command properly initialized.

3.2 Route-2

Having described Route-1, the adjustments to the `isy` file to obtain a script performing a Route-2 type of calculation are quite easy. Only a few points should be taken into account.

- The first step is to run an HF or DFT Gaussian calculation, which could be a single point energy or a geometry optimization calculation, saving the check point file.

- Transform the check point file in a formatted file.

- Run `MOMO check_point.fchk`, writing an `isy` file.

As an example, let us consider the borazine molecule and the following Gaussian input file, for a geometry optimization at the B3LYP/6-31G(d) level.

```
 1 %chk=borazine.chk
 2 # opt freq b3lyp/6-31g(d) 10f 6d
 3
 4 borazine geo opt at b3lyp/6-31g(d)
 5
 6 0 1
 7 X1
 8 X2 X1 1.0
 9 N1 X2  NX X1  90.0
10 X3 X2 1.0 N1  90.0 X1  180.0
11 N2 X2  NX X1  90.0 N1  120.0
12 N3 X2  NX X1  90.0 N1 -120.0
13 B1 X2  BX X1  90.0 N1  180.0
```

```
14 B2 X2  BX X1  90.0 B1  120.0
15 B3 X2  BX X1  90.0 B1 -120.0
16 H1 X2  HN X1  90.0 N1    0.0
17 H2 X2  HN X1  90.0 N2    0.0
18 H3 X2  HN X1  90.0 N3    0.0
19 H4 X2  HB X1  90.0 B1    0.0
20 H5 X2  HB X1  90.0 B2    0.0
21 H6 X2  HB X1  90.0 B3    0.0
22 Variables:
23 NX 1.407110
24 HN 2.409672
25 BX 1.447738
26 HB 2.643086
27
```

When the Gaussian calculation has finished, type the commands

```
prompt> formchk borazine
prompt> MOMO borazine.fchk
```

and, whitin the `MOMO` run, type

```
yxz
spg D3d
write borazine.isy
y
q
```

Then, the `borazine.isy` file should read:

```
 1 #!/bin/bash
 2 mo230xl << next
 3 BORAZINE GEO OPT AT B3LYP/6-31G(D)
 4
 5 D3H
 6 N1          2.66600150E+00    0.00000000E+00    0.00000000E+00
 7 S   6
 8 4.17351146E+03  1.83477216E-03
 9 6.27457911E+02  1.39946270E-02
10 1.42902093E+02  6.85865518E-02
11 4.02343293E+01  2.32240873E-01
12 1.28202129E+01  4.69069948E-01
13 4.39043701E+00  3.60455199E-01
14 S   3
15 1.16263619E+01 -1.14961182E-01
16 2.71627981E+00 -1.69117479E-01
17 7.72218397E-01  1.14585195E+00
18 P   3
```

```
19 1.16263619E+01  6.75797439E-02
20 2.71627981E+00  3.23907296E-01
21 7.72218397E-01  7.40895140E-01
22 S   1
23 2.12031498E-01  1.00000000E+00
24 P   1
25 2.12031498E-01  1.00000000E+00
26 D   1
27 8.00000000E-01  1.00000000E+00
28 N2  N1     -1.33300075E+00    2.30882502E+00   -6.07049125E-17
29 N2  N1     -1.33300075E+00   -2.30882502E+00    6.07049125E-17
30 B1         -2.74211085E+00    0.00000000E+00    0.00000000E+00
31 S   6
32 2.06888225E+03  1.86627459E-03
33 3.10649570E+02  1.42514817E-02
34 7.06830330E+01  6.95516185E-02
35 1.98610803E+01  2.32572933E-01
36 6.29930484E+00  4.67078712E-01
37 2.12702697E+00  3.63431440E-01
38 S   3
39 4.72797107E+00 -1.30393797E-01
40 1.19033774E+00 -1.30788951E-01
41 3.59411683E-01  1.13094448E+00
42 P   3
43 4.72797107E+00  7.45975799E-02
44 1.19033774E+00  3.07846677E-01
45 3.59411683E-01  7.43456834E-01
46 S   1
47 1.26751247E-01  1.00000000E+00
48 P   1
49 1.26751247E-01  1.00000000E+00
50 D   1
51 6.00000000E-01  1.00000000E+00
52 B2  B1      1.37105543E+00   -2.37473766E+00    6.87768824E-17
53 B2  B1      1.37105543E+00    2.37473766E+00   -6.87768824E-17
54 H1          4.57733472E+00    0.00000000E+00    8.75811540E-47
55 S   3
56 1.87311370E+01  3.34946043E-02
57 2.82539436E+00  2.34726953E-01
58 6.40121692E-01  8.13757326E-01
59 S   1
69 1.61277759E-01  1.00000000E+00
61 H2  H1     -2.28866736E+00    3.96408815E+00   -4.13715765E-17
62 H2  H1     -2.28866736E+00   -3.96408815E+00    4.13715765E-17
63 H2  H1     -5.00445550E+00    0.00000000E+00   -8.75811540E-47
64 H2  H1      2.50222775E+00   -4.33398559E+00    8.66709485E-17
```

```
 65 H2  H1      2.50222775E+00    4.33398559E+00   -8.66709485E-17
 66
 67 next
 68 if [ $? == 0 ]; then
 69 mo400xl << next
 70 BORAZINE GEO OPT AT B3LYP/6-31G(D)
 71 SODILI 1E-6 EOSCISTOP 50
 72 gaumos borazine.fchk yxz
 73
 74 21
 75 next
 76 if [ $? == 0 ]; then
 77 mo600xl << next
 78 BORAZINE GEO OPT AT B3LYP/6-31G(D)
 79
 80 momento-di-dipolo salva
 81 momento-lineare   salva
 82 momento-angolare  salva
 83
 84 next
 85 if [ $? == 0 ]; then
 86 mo690xl << next
 87 BORAZINE GEO OPT AT B3LYP/6-31G(D)
 88 HFEXCHANGE x.xx
 89
 90
 91 next
 92 if [ $? == 0 ]; then
 93 mo710xl << next
 94 BORAZINE GEO OPT AT B3LYP/6-31G(D)
 95 HFEXCHANGE 0.20
 96
 97
 98 next
 99 if [ $? == 0 ]; then
100 rm -f fort.4 fort.20
101 tar -a -cf borazine.tgz fort.*
102 rm -f fort.*
103 fi
104 fi
105 fi
106 fi
107 fi
108 exit
```

In this case also, to perform a magnetic perturbed calculation only, lines 85-91 must be deleted, as well as line 103. Now the script is ready and can be submitted to perform the

B3LYP/6-31G(d) calculation of the magnetic perturbation using the command

```
prompt> ./borazine.isy >& borazine.osy &
```

SYSMO program output files are collected in the `borazine.osy` file and `borazine.tgz` contains the FORTRAN files for the subsequent current density calculations.

Some concluding remarks for this section are as follows.

- Geometry and basis set are taken from the `fchk` file, this is the only way.
- Always using Cartesian Gaussian functions by means of the `6d` and `10f` options on the Gaussian route card.
- The `MOMO` program recognizes only a few functionals and their HF exchange fractions. Therefore, always check line 95 of the `isy` file to see whether the correct `HFEXCHANGE` value has been inserted.
- Pure functionals require `HFEXCHANGE 0` and the calculation of two-electron integrals can be skipped by inserting the string `MAXREC 0` in line 4 followed by a new blank line. In this case the calculation is very fast.
- If the Gaussian calculation is at HF level, remove line 95.

3.3 Route-3

Choosing this route, SYSMO programs are not used, since the magnetic perturbed calculation is left to Gaussian according to the following job file (the cyclooctatetraene is taken as an example, where the geometry optimized in a previous run is read from the checkpoint file `COT.chk`).

```
1 %chk=COT.chk
2 # b3lyp/6-31g(d) nmr=csgt output=(wfx,csgt) Geom=Checkpoint
3
4 ciclooctatetraene planare D4h CSGT B3LYP 6-31G*
5
6 0 1
7
8 COT.wfx
9
```

Here it is important to note that the `NMR` keyword is set equal to the Continuous Set of Gauge Transformations (CSGT). This is mandatory.

At the end of the calculation the wavefunction file `COT.wfx` contains the perturbed coefficients, which can be converted in FORTRAN files fully compatible with the SYSMO ones by means of the utility program `unpackwfx` using the command

```
prompt> unpackwfx COT
```

This command produces the files `fort.3, fort.11, fort.23`, and `fort.28` used by the IC programs 4.

4 Induced Current Density Programs

IC programs can be used to compute the current density and related properties. Before using them, the FORTRAN files `fort.3, fort.11, fort.23`, and `fort.28` should be generated. Depending on which type of route has been adopted for the magnetic perturbed calculation, see previous sections, the FORTRAN files can be generated using the command

```
prompt> tar -zxf sysmo-file.tgz     (or prompt> unpack sysmo-fsy-file)
```

or

```
prompt> unpackwfx gaussian-file.wfx
```

Examples in the following are given for benzene, planar-COT, and borazine at the B3LYP/6-31G(d) level. The full set of examples here reported plus those in the reference paper can be found here.

4.1 `JBMAP` - Current density vector map

To obtain current density maps for each orientation of the perturbing magnetic fields, the program `JBMAP` can be used either interactively

```
prompt> JBMAP [ options ]
```

or redirecting the input from a file

```
prompt> JBMAP [ options ] < somefile.txt
```

The easiest way to use the program is to type the command without options and go forward accepting defaults. In this case, the (unitary) magnetic field is parallel to the z Cartesian axis and the file `JBF.3d` is generated with the map to be visualized using the `v3d` program 4.6.
This could be enough in many a cases, in particular, for planar systems placed on the xy plane. However, defaults can be modified to consider actual cases, using on-line command options and/or during the interactive use of the program. For a list of options type:

```
prompt> JBMAP -h
-o STRING graphic file name, do not add .3d
-f FAT molecular model scale factor
-g GX GY GZ gauge origin (a.u.)
-B BX BY BZ magnetic field components
-j TOT | ROT/PARA | TRA/DIA
-m CO|DZ1|DZ2|PZ1|PZ2|GRRO,GPRO,CSGT,BS,BCP
-A GRRO/GPRO variable
-GCE STRING external grid file name
-q +-N O1 O2 ... ON: +add,-del MOs from the sum
-qf file reads +-N O1 O2 ...ON from file
-h this help
```

Most of these options depend on the flexibility of the CTOCD method and merit some attention. The `-m` option establishes the variant of the method, where some of them are more useful that others depending on the calculation type. However, it should be kept in mind that all CTOCD variants give the same result in the limit of a complete basis set calculation. For current density maps the default is `DZ2`, which is fine almost in all cases. For major details on `-m`, as well as on `-g, -j, -A, -q, -qf` options see 4.7.
The remaining options can be easily understood as discussed here below commenting the following command.

```
prompt> JBMAP -o map -f 0.1 -B 1 0 0 -GCE extgrid
```

In this example: the program generates the `map.3d` file with the graph of the current field; the thickness of the ball-and-stick molecular model is reduced to 0.1 respect to the default value of 0.3; the magnetic field is parallel to the x Cartesian axis. It should be considered that even if the three components of $\mathbf{B}$ can be typed freely, the program always normalizes them to obtain a unitary perturbing field. The `-CGE` option permits to read an external grid of current density values from file `extgrid`. The `extgrid` text file contains Nato + NPoints lines. The first Nato lines have the format:

```
AtomSymbol X Y Z
```

The NPoints lines have the format:

```
x y z Jx Jy Jz
```

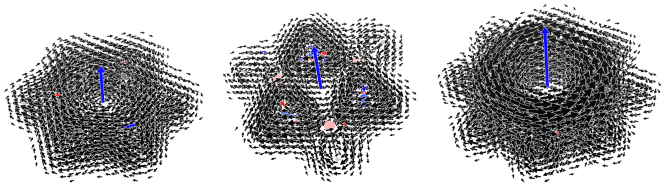
During the interactive use, the program prints:

```
-------------------------------------------------------
FRE3D
magnetic field.........B    0.0000    0.0000    1.0000
gauge origin...........G    0.0000    0.0000    0.0000
comp 0=p+d,1=p,2=d.JTERM    0
method 0,1,2,3,4....METH    2
lower vertex..........RI   -6.0639   -6.6926   -2.0000
upper vertex..........RF    6.0639    6.6926    2.0000
cutoff min/max.......FMM    0.0200    0.1000
arrow fatt a0/J.....FATT    8.0000
arrow density.......STEP    0.6000
J.B>J*frac color....FRAC    1.0000
0=length,1=area.....LUNA    1
ok? [s]
-------------------------------------------------------
```

and waits for some reply. The magnetic field components and the CTOCD details can be changed once again, but what matter here is the possibility to change the exploration space, as well as the cutoff filters, the arrow size and density. To make changes, type the proper key followed by a value, for example

```
RI -6 -5 1
RF  7  4 1
FMM 0.05 1.5
FATT 10
STEP 0.4
FRAC 0.3
LUNA 0
```

These: to fix the exploration space to a plane at 1 au above and parallel to the xy plane, extending from -6 to 7 au along x and from -5 to 4 au along y; to set the cutoff filters to 0.05 and 1.5 au for the minimum and maximum current density vector module, respectively; to set a scale factor of 10 for the arrow size; to set a step of 0.4 au between grid points; to set to 0.3 the fraction of the current modulus along **B** to have arrow colors in red/blue if the fraction is parallel/anti-parallel to **B**. When `LUNA` is set to 0/1, arrow length/area is proportional to the modulus of the current density. When everything is ok, press the return key to complete the calculation. Collecting all these values in `somefile.txt` and redirecting the input from this file, is very useful to fix standard values to compare the maps of different molecules.
Examples of current density maps for benzene, borazine and planar cyclooctatetraene generated by `JBMAP` are shown in the following. Instructions and commands to calculate the maps here exposed can be found here.



4.2 `BOCUST` - Bond current strength

To obtain bond current strengths for each orientation of the perturbing magnetic fields, the program `BOCUST` can be used either interactively

```
prompt> BOCUST [ options ]
```

or redirecting the input from a file

```
prompt> BOCUST [ options ] < somefile.txt
```

The easiest way to use the program is to type the command without options. The program prompts for any pair of atoms found at a distance between the default values `DISTMIN` and `DISTMAX`. Replying `y/Y` the atom pair is selected for the current strength calculation, else the atom pair is skipped. Type `N` to exit immediately the calculation.
Sometime the list of atomic pairs could be relatively long. Therefore, preparing `somefile.txt` with one `y/n` per line could be useful in case to repeat the calculation with different options. In either case, a file `BCS.3d` is generated containing visual information about the calculated current strengths. It can be visualized using the `v3d` program 4.6.

The current strength `CS` is reported for each atomic pair in the output with the following format

```
 CONTRIBUTION  1 -0.5297042E+00 AU -0.1492675E-07 SI
 CONTRIBUTION  3  0.1773644E+00 AU  0.4998022E-08 SI
 TOTAL CS ==>    -0.3523398E+00 AU -0.9928726E-08 SI
 CS/CS0 ratio     0.83
```

where contributions are reported for each min/max of the current density cross section. The sum of contributions is given by `TOTAL CS`, which is the *net* bond current strength. Contributions and total are reported in atomic and SI units. The program uses a reference current strength `CS0` (by default `CS0`=12 nA/T) and prints the ratio `CS/CS0` after the `TOTALE`. The ratio×100 is reported also on the graphic file. For a better comparison it is suggested to use the net bond current strength calculated for a benzene C-C bond using same method and basis set.

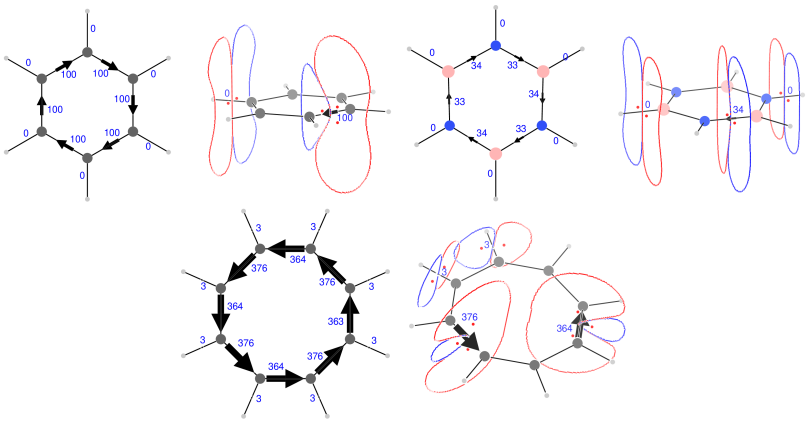
Defaults can be modified to consider particular cases using on-line command options. For a list of options type:

```
prompt> BOCUST -h
-o STRING graphic file name, do not add .3d
-f FAT molecular model scale factor
-g GX GY GZ gauge origin (a.u.)
-B BX BY BZ magnetic field components
-j TOT | ROT/PARA | TRA/DIA
-m CO|DZ1|DZ2|PZ1|PZ2|GRRO,GPRO,CSGT,BS,BCP
-A GRRO/GORO variable
-GCE STRING external grid file name
-q +-N O1 O2 ... ON: +add,-del MOs from the sum
-qf file reads +-N O1 O2 ...ON from file
-h this help
-----------------------
-p DELTA grid step (a.u.)
-x DIM OFFSET horizontal cross-section size (a.u.)
-y DIM OFFSET  vertical  cross-section size (a.u.)
-d DISTMIN minimum interatomic distance   (Ang)
-D DISTMAX maximum interatomic distance   (Ang)
-e VALORE contour level of integration domain (a.u.)
-emm VALORE min/max search criterion
-P FAT plot J as balls proportional to FAT
-C SPS plot line frame thickness proportional to SPS
-l 1,2,3,... progressive contour levels, if 999->3D
-I SPS ntegrate full frame, border line thickness=SPS
-CS0 REF reference current strength nA/T
-nocd dont plot points and domain contours
```

Up to `-h`, options are the same as for the `JBMAP` program 4.1. In particular the CTOCD details are described in 4.7.
Other options can be used to change: the grid grain (`-p`), the cross section rectangular size and its offset respect to the atomic pair center (`-x`, `-y`); the min and max distance between atoms to select atomic pairs (`-d`, `-D`); the value of the contour level which is

used as integration domain (`-e`); the integration domain from contour levels to the full cross section (`-I`); the reference current strength (`-CS0`).

Examples for benzene, borazine and COT molecules are provided here in the following. Benzene computed at the same level of theory and basis set, has been chosen as a reference for all the molecules. Diatropic/paratropic circulations are clockwise/anticlockwise. At this level, borazine shows a sizable net diatropic ring current, whilst in COT the two C-C bond sustain a paratropic current which is nearly four times larger than the reference. The net current strengths for the X-H bonds is vanishing for benzene and borazine; for COT a very small current strength can be observed consistent with adjacent bay ring currents. Instructions and commands to generate the examples can be found here.



4.3 `STAGRA` - Stagnation graph

To obtain a stagnation graph (GS) for each orientation of the perturbing magnetic fields, the program `STAGRA` can be used either interactively (suggested way)

```
prompt> STAGRA [ options ]
```

or redirecting the input from a file (less frequently)

```
prompt> STAGRA [ options ] < somefile.txt
```

The easiest way to use the program is to type the command indicating the magnetic field components by means of the option `-B` $\texttt{comp}_x$ $\texttt{comp}_y$ $\texttt{comp}_z$ (by default the magnetic field is set to `-B 0 0 1`). The program starts searching for singularities of the current density over planes perpendicular to the magnetic field in steps set by the option `-step_B` `some_value_in_au` (by default `some_value_in_au` is equal to 0.2 au). The dimensions of the searching field is determined automatically by the program on the basis of the atomic coordinates. However, the searching field can be changed using the options `-x` x_{min} x_{max}, `-y` y_{min} y_{max}, and `-z` z_{min} z_{max} (the order is not mandatory). For every singularity found, the program writes a line having the following format

`|` `SP X Y Z (`r`,`s`)` ξ_1 ξ_2 ξ_3

where the stagnation point `SP` can be either `Para`, `Dia`, or `Sel`, which stand for paratropic center, diatropic center, or saddle point, respectively; `X Y Z` are the coordinates (in au) of the singularity; (r,s) are *rank* and *signature* of the singularity; ξ_1 ξ_2 ξ_3 are the eigenvalues

of $\left(\nabla_\beta J^{\mathbf{B}}_\alpha\right)_{\mathbf{r}_0}$, i.e., the Jacobian of the induced current density calculated in the stagnation point $\mathbf{r}_0$. A file `GS.3d` is generated containing the meta-graphic of the stagnation, which can be visualized using the `v3d` program 4.6.

For a list of options type:

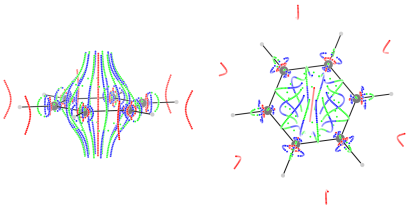
```
prompt> STAGRA -h
-o STRING graphic file name, do not add .3d
-f FAT molecular model scale factor
-g GX GY GZ gauge origin (a.u.)
-B BX BY BZ magnetic field components
-j TOT | ROT/PARA | TRA/DIA
-m CO|DZ1|DZ2|PZ1|PZ2|GRRO,GPRO,CSGT,BS,BCP
-A GRRO/GPRO variable
-q +-N O1 O2 ... ON: +add,-del MOs from the sum
-qf file reads +-N O1 O2 ...ON from file
-h this help
-----------------------------------
-2D set J parallel to B to zero (pseudo-SG)
-x XMIN XMAX  window size along x
-y YMIN YMAX  window size along y
-z ZMIN ZMAX  window size along z
-hx XSTP  exploration step for x
-hy YSTP  exploration step for y
-hz ZSTP  exploration step for z
-stepB VAL updates ZSTP along B direction
-eps EPSI Newton-Raphson minimum criterion
-itm ITMAX Newton-Raphson max iterations
-pgm SPMAX Stagnation Graphic max points
-drd DMIN minimum distance among singulatities
-sgs STRING stagnation graph saving file (XX=nosave)
-lgs S1-S2-...Sn: stag-graph reading files (XX=noread)
-crc S T size and thickness saddle crosses (S<0 dots)
-rgp R dots-radius for centers (and saddles)
-por D saddle connection graph d=SP-trajectory dist.
-v set verbose printing to 0(min), 1(SG-point), 2(max)
```

Up to `-h`, options are the same as for the `JBMAP` program 4.1. In particular the CTOCD details are described in 4.7.
Other options can be used to change: SG to pseudo-SG (`-2D`); dimension of the searching field (`-x`, `-y`, `-z`); steps of search (`-hx`, `-hy`, `-hz`, `-stepB`); Newton-Raphson criterion and maximum number of iterations (`-eps`, `-itm`); maximum number of stagnation points (`-pgm`) and their inter-distance (`-drd`); file name for saving the stagnation graph (`-sgs`); file name for reading the stagnation graph (`-lgs`); size and thickness of the crosses indicating the saddle positions (`-crc`); radius of the dots indicating the center positions (`-rgp`); saddle connection graph calculation from off to on (`-por`); type of output (`-v`).

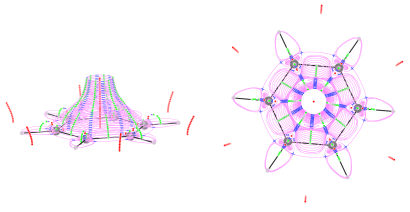
Further hints.

- When using the `-lgs` option the stagnation graph is not calculated, it is read from the specified file (or list of files).
- different portions of a stagnation graph can be searched separately and eventually written on a file, let say `fnp1, fnp2,...fnpn` for file-name-portion-1, file-name-portion-2 and so on.
- All different files can be read together using `-lgs fnp1-fnp2-...-fnpn` to obtain the full stagnation graph.
- To calculate a *true* SG, it is suggested to perform first a pseudo-SG calculation using `STAGRA -2D -sgs psdfn` (to save the pseudo-SG on the `psdfn` file); then run `STAGRA -lgs psdfn` (note the absence of the `-2D` option in the second run).
- When using the `-por` option to calculate a saddle connection graph (SCG), let say `STAGRA -por 0.1`, note that the value (0.1 au) sets the distance between the saddle position and the starting point of the induced current density trajectory; at the same time it sets also the distance for a connection with another saddle (which may also be a different arm of the same starting saddle).
- Whit the `-por` option the program prompts once to change the vertices of the molecular space in which to confine the trajectory (by default these are the same of the searching field and are good almost always), twice to change many subtle technicalities such as the trajectory integration method (by default a 4th order Runge-Kutta is used), the possibility to show a small direction arrow along the trajectory and many other things, which is better to skip over in many occasions.

Examples for the benzene molecule are provided here in the following. Instructions and commands to generate the examples can be found here.



Two views of the same pseudo-stagnation graph.



Two views of the same saddle connection graph.

4.4 `FIELD` - Density functions

A number of density functions related to the current density tensor can be calculated using the program `FIELD`. A list of the available densities can be obtained issuing the command

```
prompt> FIELD -h
usage: FIELD [verbo] P1 [para-opz]
verbo makes a verbose output
P1 is mandatory and must be one of the following:
RHO electron density
GRAD_RHO electron density gradient module
GRAD_RHONUM numerical GRAD RHO
LAPL_RHO electron density Laplacian
ACID   Current Density Tensor (T) anisotropy (Herges)
VARt   variance Var(t)=sigma^2(t),  t=eigenvalues(T)
SIGt   std deviation sigma(t)
PVART  pseudo-variance: pVar(T)=tau(T)
VARTS  variance of the symmetric part Var(TS)
SIGTS  std deviation symmetric part sigma(TS)
VARTA  variance of the anti-symmetric part Var(TA)
SIGTA  std deviation anti-symmetric part sigma(TA)
TRT    trace(T)
DETT   determinant of T
AVT    anisotropy of the Vorticity Tensor (V) Pel.Laz.
TVCD   trace of the vorticity tensor (Barquera-Lozada)
DETV   determinant of V
MO     molecular orbital value
DIV_J  divergence of the induced current density (IC)
DIV_JN divergence of IC numerical
MSD_ij magnetic shielding density at R_I ij component
Optional pameters - to change defaults type:
...
...
```

Actualizing the first parameter `P1` with one of the listed keywords, the corresponding density function will be calculated and ready to be displayed. The main result is a graphic representation of the selected density. By default a 3D isosurface will be produced, but also 2D representations by means of contour levels or divergent color maps can be obtained. Different choices can be tuned using the optional parameters listed below.

```
Optional pameters - to change defaults type:
-o STRING graphic file name, do not add .3d
-f FAT molecular model scale factor
-g GX GY GZ gauge origin (a.u.)
-B BX BY BZ magnetic field components (pristine)
-BU BX BY BZ mag-field components to make unitary
-j TOT | ROT/PARA | TRA/DIA
-m CO|DZ1|DZ2|PZ1|PZ2|GRRO,GPRO,CSGT,BS,BCP
-A GRRO/GPRO variable
-q +-N O1 O2 ... ON: +add,-del MOs from the sum
-qf file reads +-N O1 O2 ...ON from file
-h this help
```

```
-----------------------------------
-v VAL contour surface value (a.u.)
-p DELTA grid step (a.u.)
-s TYPE surface type:0-curliv;1-cloud;2-cloud;3-curliv
-x XMIN XMAX  window size along x (au)
-y YMIN YMAX  window size along y (au)
-z ZMIN ZMAX  window size along z (au)
-c COLOR of the surface (26-32)
-t THICKNESS of contour levels
-l SCALING of contour levels (if 0 no contours)
-e EPSI minimum contour level value
-% PERC max/min percentage for the first contour
-DCM MIN MAX Diverging Color Map (0 0 for cube_minmax)
-R_I X Y Z coord magnetic shielding density reference
```

Up to `-h`, options are the same as for the `JBMAP` program 4.1. In particular the CTOCD details are described in 4.7.
Other options can be used to change the isosurface value (`-v VAL`), or the exploration space size (`-x XMIN XMAX, -y YMIN YMAX, -z ZMIN ZMAX`). In particular, when the space is restricted to be a plane, i.e., when one of the `MIN`'s is equal to the corresponding `MAX`, the program produces a 2D graph on that plane instead of the default 3D isosurface. The 2D graph can be produced as a contour levels or a divergent color map or both. Contour levels are switched on using `-l` with a `SCALING` not equal zero. Divergent color maps can be obtained using the `-DCM` option.

Further hints.

- Sometime the calculation of the cube of values can be very time consuming and even an apparently simple change of some of the parameters could result in a boring repetition of a long calculation. Therefore, at the end of the cube calculation, the program prints the actual values of the parameters controlling the graphic and prompts for their change. Before to exit pressing `<q>` on the keyboard, it is convenient to open the graphic file using the `v3d` program and check the result. Eventually, some parameter can be changed and the graphic seen again, until a satisfactory result is obtained.

- For field having both positive and negative regions, `FIELD` does not use the isosurface value set by the `-v` option, instead it prompts in real-time for two new values.

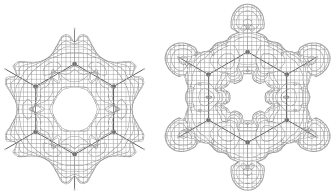
- The grid grade can be changed using `-p` where `DELTA` is the grid step in a.u..

- A color for the isosurface can be set using `-c` followed by `26=red`, `27=green`, `28=blue`, `29=cyan`, `30=magenta`, `31=yellow`. The default value is `32=black`. When a field can have both positive and negative values, two complementary colors will be used.

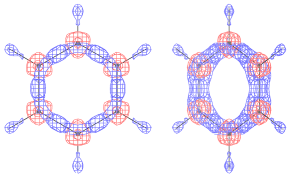
- Contour level `THICKNESS` can be changed using the `-t` option.

- Contour level `SCALING` can be changed using `-l`, where `SCALING` is the ratio between successive contour values, starting from a percentage (`PERC`) of the field maximum value, scaled up to a minimum value set by `-e EPSI`.
- The magnetic field (see `-B BX BY BZ`) is used only to compute the divergence of the induced current density.

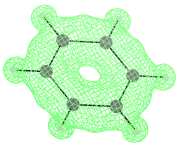
Instructions and commands to generate the examples provided in the following for the benzene molecule can be found here.



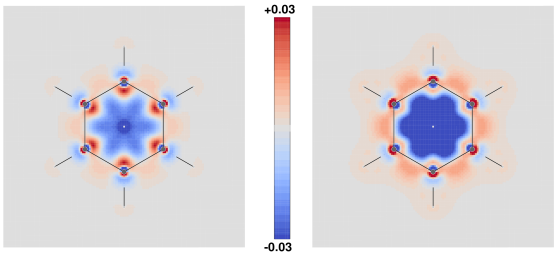
ACID isosurface for a value of 0.05 a.u. on the left and AACID isosurface for a value of 0.02 a.u. on the right.



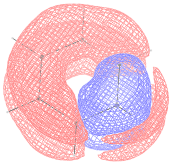
Two views of the Trace of the Vorticity of the Current Density tensor (TVCD). Isosurface values are -4.2E-3 (blue) and 2E-3 (red) a.u..



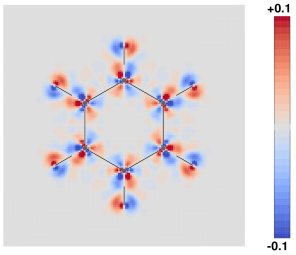
Anisotropy of the Vorticity Tensor (AVT). Isosurface value is 0.01 a.u..



Divergent color map of the magnetic shielding density at the center of mass: average value on the left; perpendicular component on the right.



The π-electron contribution to the parallel component of the proton magnetic shielding density. Isosurface values are -1E-4 (blue, deshielding) and 1E-4 (red, shielding).



Divergent color map of the divergence of the current density vector induced by a perpendicular magnetic field.

4.5 JECK - Point by point

The package provides a basic program (JECK) to calculate the current density tensor and its geometrical derivatives for any grid of points, with freely chosen size and step. This will allow people to use their own methods to obtain the induced current density, derive further quantities and/or apply different visualization techniques. The program can be used interactively through an intuitive interface, which appears after having invoked the program as

```
prompt> JECK
```

the interface is displayed on the screen as

```
Program JECK - Feb 13, 2020 - 13:45
************************************************
Q =  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
CTOCD =     1
JTERM =     0
CO    =     0.0000000    0.0000000    0.0000000
B     =     0.0000000    0.0000000    1.0000000
MIN   =     1.0000000    1.0000000    1.0000000
MAX   =     1.0000000    1.0000000    1.0000000
STEP  =     1.0000000
H     =     0.0001000
DERIV =     F
R2D   =     F
ALFA  =     2.0000000
VERBO =     F
GR XXXX compute the grid and write it on XXXX file
E to exit
```

The program reads anything and look for:

`Q` Select which occupied MO's are in the sum, it must be followed by $n+1$ values, the first indicating the number of MO's, the remaining are the MO canonical indices

`CTOCD` followed by an integer, choses the CTOCD variant 4.7

`JTERM` 0=total, 1=para, 2=dia

`CO` Common Origin coordinates

`B` Magnetic field components

`MIN` Lower grid corner

`MAX` Upper grid corner

`STEP` grid step

`H` incremental for numerical derivatives

`DERIV` Derivatives on/off

`R2D` Point to origin displacement on/off

`ALFA` Costant for GRRO/GPRO

`VERBO` Verbose printing

`GR` The grid is computed and written on the XXXX external file

Issuing an empty line makes the grid values to be computed and displayed on the screen. This last way is recommended for very small grids or to check the current density tensor and vector values for one single point, which can be selected entering the three coordinates of `MIN` equal to those of `MAX`. Switching on `DERIV`, analytical and numerical derivatives of the current density vector, for the magnetic field issued through the `B` parameter, will be displayed. Changing the incremental parameter `H` one can see how numerical derivatives approaches analytical ones.

For large grids the `GR XXXX` command generates the `XXXX` file containing the current density tensor values for each point of the grid. If `DERIV` is true, then also analytical derivatives of the current density tensor are written on the file, which starts with a brief preamble describing how the data were written and, consequently, how they can be read.

4.6 `v3d` - Visualization of 3D graphic files

Files with extension `3d` or `v3d`, generated by the SYSMOIC programs, are meta-graphic files, which can be visualized using the `v3d` program by typing

```
prompt> v3d graphic-metafile.3d [-npix window-size]
```

Aside the terminal, a new window appears displaying the graphic. Mouse can be used as usual, plus a number of other keyboard commands, whose meaning is described on the terminal once pressing the `<h>` key. Most useful are: `<p>` to write a PostScript file with the visualization present on the graphic window; `<e><p>` to write En-capsuled-PS file; `<S>` to write the `SpecialValue.txt` file with the current status of the point-of-view, scale factor, contour spacing, fog and so on.

4.7 CTOCD setting

`-m` Set the CTOCD variant:

- `CO` common origin, the constant components of the displacement vector $\mathbf{d}$ are set by the `-g` option, the default value is 0,0,0;
- `DZ1` diamagnetic zero, in this case the displacement vector is set to the point in which the current density is computed, $\mathbf{d} = \mathbf{d}(\mathbf{r}) = \mathbf{r}$, see KB, LMZ;
- `DZ2` as `DZ1` with weighted shift of the origin toward the nearest nucleus, see KB, FZCS;
- `PZ1` paramagnetic zero, the displacement vector is set to a point for annihilating the components of the current density perpendicular to $\mathbf{B}$, see ZLMP;
- `PZ2` as `PZ1` with weighted shift of the origin toward the nearest nucleus, see Z;
- `GRRO` after the GRadient of RhO, see BMZ
- `GPRO` after the Gradient and a Power of RhO, see BMZ
- `CSGT` after the Continuous Set of Gauge Transformations, see CTKF
- `BS` as CSGT with atomic size adjustments using empirical atomic radii of Bragg and Slater, see B
- `BCP` as CSGT with atomic size adjustments using atomic radii obtained from the bond critical points determined by the electron density distribution, see MSZ

`-g` Relevant only when `-m CO`, with the component of the origin displacement vector, by default is 0,0,0.

`-j` Choose which component among diamagnetic, paramagnetic and total of the current density vector is computed. When `-m DZ1`, diamagnetic=transnational and paramagnetic=rotational. By default is 0 (Total).

`-A` Relevant only when `-m GRRO/GPRO`, with the constant of the method, by default is -0.0748 (optimized value for the GPRO, see BMZ).

`-q` Select which occupied MO's are in the sum, it must be followed by $n+1$ values, the first indicating the number of MO's, the remaining are the MO canonical indices. When the number of MO's is negative, the MO's are deleted from the total sum. In addition to symmetry labels, a symmetry classification of the orbitals can be obtained running TIPOMO.

`-qf` Followed by a file name, the same as `-q` with the $n+1$ values read from the file.