

# User's Guide to DAMQT 3.2.0

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DAMQT 3.2.0

DAMQT is a package for the analysis and visualization of the molecular electron density (MED) in atoms and molecules, and several related properties like density deformations, electrostatic potential, molecular topography, sigma holes, electric field, Hellmann-Feynman forces, molecular orbitals and density finger-prints in Zernike-Canterakis and Jacobi functions. Furthermore, cluster optimization for non-bonding interacting systems has been recently added to the package.

The method used is based on the DAM partition of the electron density into atomic fragments by means of a least deformation criterion described elsewhere<sup>1</sup>. On the other hand, density fingerprints are computed as expansions of Zernike-Canterakis or Jacobi functions inside a ball of user-supplied radius using translation techniques of Slater or Gaussian basis functions<sup>2</sup>. Cluster optimization is carried out by means of the EPIC procedure (Gadre S, Babu K Resonance 4 (1999) 40).

In the DAM partition, the electron density of every atomic fragment is expanded in products of radial factors times regular spherical harmonics centered at its nucleus. The electron density of the full molecule is thus represented as a set of atomic expansions in terms of effective multipoles, which are functions of the distance to their corresponding nuclei.

The radial factors of the effective multipoles are piecewise expanded in terms of exponentials times polynomials of variable  $r$ . This representation is used for the fast evaluation of the molecular electrostatic potential (MESP) and field generated by the electron density and nuclei, and for the computation of the Hellmann-Feynman forces on the nuclei as well. The molecular topography of MED and MESP, and the atomic and molecular deformations of density can be also depicted, yielding a picture that connects with several concepts of the empirical structural chemistry.

DAMQT has a modular structure in three levels (see fig 1), with the interfaces to standard packages for quantum mechanical calculations placed on top. In case of ADF, although the interface is available in the suite, we also include it as part of DAMQT for completeness. Interfaces to MOLPRO, GAUSSIAN, MOPAC, TURBOMOLE and NWChem are currently included in the package, as well as a facility to read MOLEKEL *.mkl* files.

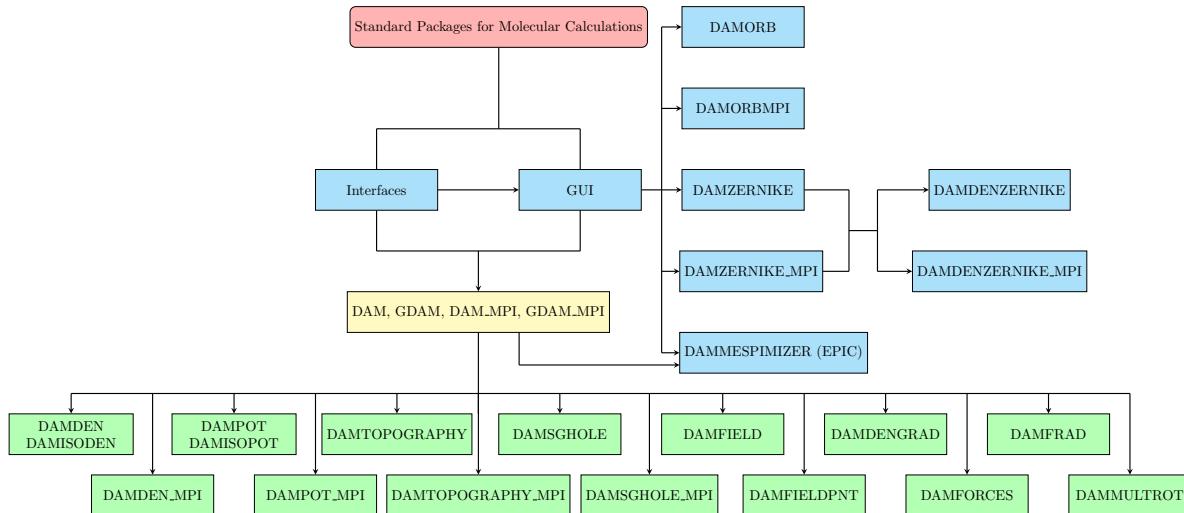


Figure 1: DAMQT structure

In this level too, DAMQT includes the GUI designed to facilitate usage. This GUI is written in C++ and

<sup>1</sup>For a description of the fundamentals, see for instance, J. Fernández Rico, et al. Comput. Chem. 25 (2004) 1355; J. Mol. Struct. Theochem 727 (2005) 115, and the references included in these articles

<sup>2</sup>For details see G. Urquiza-Carvalho et al. J. Comput. Chem. 39 (2018) 2022.

has been developed using Qt library<sup>3</sup>, to facilitate portability between different operating systems. Also in this level there are some programs available for generating grids of molecular orbitals for 2D plotting and 3D visualization with the GUI. Programs for Zernike-Canterakis or Jacobi expansions of MED and their grid generation for plotting appear also in this level, as they can be launched from the GUI without requiring partition/expansion of MED. Finally, cluster optimization by EPIC procedure (MESPIMIZER) is implemented within the 3D viewer, albeit it requires DAM partition/expansion for host molecule.

Second level corresponds to the programs which carry out the DAM partition/expansion of density for Gaussian and Slater densities. They are available both for scalar and parallel computation with MPI. One of these programs must be run before accessing those of the third level, because the latter needs the partition/expansion data generated by the former.

Finally, bottom level contains a variety of programs for computing several properties using DAM partition/expansion. In particular, this expansion facilitates the effective computation of electron density and its deformations, electrostatic potential, electric field, density gradient, molecular topography of electron density and electrostatic potential, sigma holes and Hellmann-Feynman forces on nuclei.

Unless otherwise explicitly stated, atomic units will be used throughout this document.

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<sup>3</sup>The Qt Company, [www.qt.io](http://www.qt.io)

# 1 Installation

DAMQT 3.2.0 is supplied for Linux and MS Windows under GNU's GPL license. The package includes the code sources as well as other ancillary files). Sources can be modified and distributed according to GPLv3 terms.

The minimum requirements for installation are 200Mb of RAM memory and 150Mb of disk storage. Memory requirements strongly depend on the size of the systems to be treated. Access to Fortran 90 and C++ compilers and a python interpreter is also required.

Qt-project's Qt library 5.9 or higher (including development libraries), and OpenGL 3.3 or higher must be installed for the Linux version.

`OpenBabel` will be required for cluster optimization using openbabel atom charges.

`ffmpeg` may be necessary for creating movies from captures.

## 1.1 Linux and MacOS installation

DAM\_3.2.0 is distributed as a tarball (*DAM\_3.2.0\_datetimestamp.tar.gz*), where *datetimestamp* is an eight-digit date with format *yyyymmdd*. To install it in Linux, Unix or MacOS, enter a suitable directory and copy file *DAM\_3.2.0\_datetimestamp.tar.gz* therein. Extract the content with

```
tar -vxzf DAM_3.2.0_datetimestamp.tar.gz
```

A directory, *DAM\_3.2.0*, will be created containing the sources and ancillary files. DAM\_3.2.0 is prepared to be installed with `cmake`, therefore, check that `cmake` is already available in your system before starting installation. It can be very useful to have the graphics interface of `cmake`, named `cmake-gui`, as it greatly facilitates the handling of variables setting.

To prevent that files generated by `cmake` will be placed in the directory of DAMQT sources, it is highly recommendable to create a suitable directory and perform installation therein.

For installation with `cmake` from the command line, move to the directory where installation is desired and run either `cmake damdir` (where *damdir* is the root directory of DAMQT), or preferably, run interactively with `cmake -i`, for customization options.

By default, `make install` will install the package's files in `/usr/local/bin`, `/usr/local/man`, etc (you may need root privileges for this operation). You can specify an installation prefix other than `/usr/local` by setting `cmake` variable `CMAKE_INSTALL_PREFIX` to *path*, where *path* stands for the desired final location. (WARNING: avoid blank spaces in the pathname).

Many other installation options can be chosen by setting suitable `cmake` variables.

The package can be uninstalled with `make uninstall`.

In some systems, if `MESA` library is to be used for OpenGL, it may be necessary to run in advance the command:

```
MESA_GL_VERSION_OVERRIDE=4.5 MESA_GLSL_VERSION_OVERRIDE=450 path to DAMQT
```

in the console where DAMQT is to be launched. If a version other than 4.5 (but higher or equal to 3.3) is to be used, modify the command accordingly (change both 4.5 and 450 in the command).

## 1.2 Windows installation

MS-Windows version can be also installed with `cmake`, but an autoinstall *DAMQT\_3.2.0-setup.exe* file is also supplied with the package, so that you have only to click on this file and follow the installer instructions.

Samples folder will be installed in the *AppData/Local* folder. To prevent unwanted data losses, this folder will not be removed upon uninstalling DAMQT. It should be removed by hand if required.

To use cluster optimization with openbabel atom charges, `OpenBabel` package must be installed and the pertaining executable must be accessible. Include the directory containing the executable in the user's `PATH`, and beware that the `BABEL_DATADIR` variable is included among the user's environment variables.

Check that it points to the suitable folder (*qeq.txt* file must be present therein). An OpenBabel-3.1.1 installer is included in the directory *windows* of the package for completeness.

It is important that OpenBabel is installed and the pertaining environment variables must be set before launching a DAMQT session for cluster optimization. Otherwise, the executable or some auxiliary files will not be found and optimization may fail.

To create movies from captures, check that `ffmpeg` or any other suitable program is accessible by including the pertaining folder in the user's `PATH` variable.

### 1.3 Starting DAMQT

To start DAMQT open a *console* (UNIX/ linux/ MAC-OS) type **DAMQT320.exe** and press *enter*. In case of MS-Windows, the installer allows you to put an icon on the console for direct access. Alternatively, you can run the **DAMQT320.exe** in the installation folder.

A pop-up window will appear over a splash image (fig 2) and you will be asked to select the language. Check the option of your choice and press the *Start* button. The splash image will glow while DAMQT starts. Once the image disappears, DAMQT is ready to work.



Figure 2: Starting window

## 2 The Graphical User Interface I: Main window

The GUI has a standard design with a menu bar and a toolbar on top, an application driving menu on the left, a display area for applications standard outputs, and a menu on the right for handling graphical viewers (fig. 3).

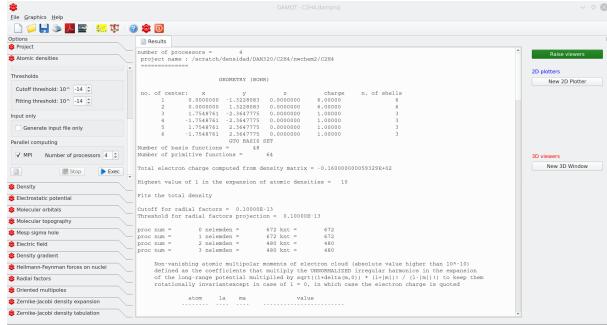


Figure 3: DAMQT main window



Figure 4: DAMQT toolbar

The toolbar (fig. 4) contains common options for this program, namely:

- New file** Clean all options to start working in a new project
- Open project** Open an existing project
- Save project** Save the current project
- Print** Send the content of the *Results* panel to the selected printer
- Pdf file** Print the content of the *Results* panel to a pdf file
- External program** Launch external program
- 2D viewer** Launch 2D viewer
- 3D viewer** Launch 3D viewer
- Help** Show this manual
- About** Show some information about the program
- Exit** Exit the program

The driving menu on the left of the main window is used for calling the different modules of DAMQT, and its contents and usage are described in this section.

Graphical tools can be launched from the toolbar or from the menu placed on the right by pressing the buttons *New 2D Plotter* or *New 3D viewer*. When graphical tools are being used, entries for the currently open 2D and 3D viewers will be displayed to facilitate navigation through them. Each open viewer has

three buttons labeled as *Raise*, *Hide*, and *Delete*. Pressing the button *Raise* the viewer will be put on top of display. The button *Hide* toggles viewer's hide and show states. Button *Delete* removes the viewer and all its content. The full set of open viewers can be raised to the foreground by pressing the button labeled as *Raise all viewers* on top of the menu.

## 2.1 Project

Every project requires files with data coming from an LCAO calculation at any level of computation. One file is necessary in all cases with extension *.ggbs* (for GTOs) or *.sgbs* (for STO), containing the geometry, nuclear charges and basis set. When DAM partition/expansion is required, another file with extension *.den*, must contain the elements of the density matrix (lower triangle). DAMQT also admits *.den* files compressed with gzip for storage saving (an extension *.den.gz* will be expected in this case) as well as binary files with density sparse matrices containing only non-null elements of the lower triangle with the format  $i, j, \rho_{ij}$ , the extension in this case being *.densprsbin*.

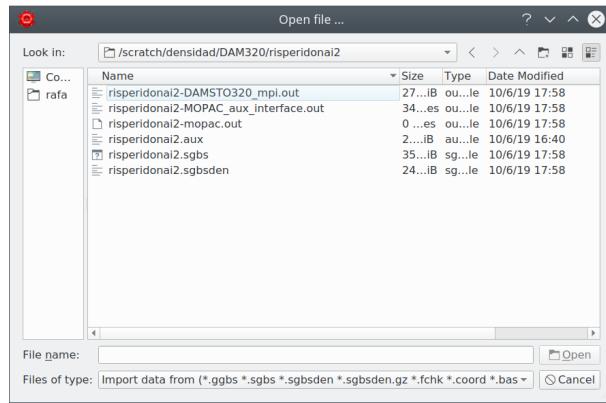


Figure 5: Import file navigator

Files *.ggbs* , (*.sgbs*) and *.den*, *.den.gz* or *.densprsbin* can be loaded by supplying their full name (including path) in the box labeled *Import data from*. Alternatively, the name of a GAUSSIAN<sup>4</sup> *.fchk* file, a MOLEKEL file *.mkl*, a TURBOMOLE basis set, coords or molecular orbitals file, *.basis*, *.coords*, *.mos* (they must be renamed to a common name with the pertaining extensions), a MOLPRO output file, *.out*, or *.xml* file, a NWCHEM output file, *.nwcout*, a MOPAC *.aux* file, or a PSI4 *.psiauxden* file can be supplied. In each case, a suitable built-in interface included in the package will automatically generate the *.ggbs* and *.den* files from output files of the corresponding package. See section 5 (*Interfaces*) in this manual for details. Pressing the key , a window is displayed for navigating through the directory tree

(see fig 5) and selecting any of these files.

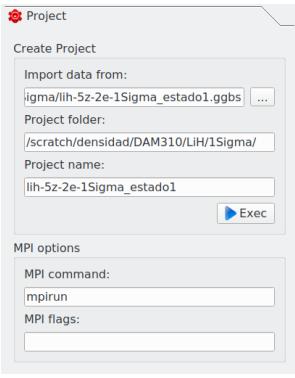


Figure 6: Project

Table 1: Suitable file extensions for running interfaces

interface	extensions
GAUSSIAN	*.fchk
MOLEKEL	*.mkl
MOLPRO	*.out, *.xml
MOPAC	*.aux
NWCHEM	*.nwcout
PSI4	*.psiauxden
TURBOMOLE	*.basis, *.coords, *.mos

**WARNING:** the current version of DAMQT only works with **spherical functions**. This is specially important in case of Gaussian basis sets, which must be spherical, not Cartesian. This implies, for instance, that if molecular calculations are to be done with GAUSSIAN, the options  $5d, 7f$  must be set in the input file.

Alternatively, the *.ggbs* and *.den* files can be hand-written following the prescription of appendix A. Further interfaces to other standard packages may be implemented in future versions.

Project files will be allocated in the folder quoted in the *Project folder* (see fig 6), and the application tentatively will assign a name to the project equal to that of the *.ggbs* or *.sgbs* files, but this can be changed by supplying an alternative name in the box labeled as *Project name*. All the files generated in the project will share the project name, unless stated otherwise in the modules menus.

To run one of the interfaces, just select a suitable file, according to the extensions shown in table 1.

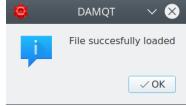


Figure 7: Project upload



Figure 8: Project opening

If an existing *.ggbs* or *.sgbs* file is selected, a message like that shown in fig 7 confirming or denying the upload will appear, followed by other confirming project opening (fig 8).

Once the required files are found, the key must be pressed for either building the *.ggbs* (*.sgbs*) and *.den* files with the interfaces to standard packages or loading them if they already exist. At the same time, a file with extension *.damproj*, which contains the default values for running the remaining modules, will be created. This process must be carried out at least once for each project.

To load an existing project, either push the icon in the toolbar or, alternatively, choose the *File* → *Open project* option in top menu, navigate to the desired project and select one of the files displayed. Recent projects can be directly accessed also from the *File* folder in top menu.

For systems with *mpi*, two boxes will appear to specify the command for executing *mpi* programs and suitable *mpi* flags (see fig 6). DAMQT checks if *mpirun* or *mpiexec* commands are installed in the system (in that order), and if any, it fills the *MPI command* box with the one found in first place.

<sup>4</sup>[www.gaussian.com](http://www.gaussian.com)

## 2.2 Atomic densities

The tab in the driving menu labeled *Atomic densities*, invokes the DAMSTO or DAMGTO programs which compute the atomic expansion of the density, the cornerstone of DAMQT partition/expansion, as shown in fig 1. One of these programs must be run at least once for every project, except for molecular orbitals plotting, or Zernike-Canterakis or Jacobi expansions. The package includes also a version of these programs for parallel computing with *mpi*.

To facilitate the computation in installations where parallel programs only can be batch processed, or in case that the user prefers to run the programs for density partition and fitting outside DAMQT environment, an option is available for only generating the input file.

The exponents and coefficients for the piecewise representation of the radial factors are stored in a file with extension *\_2016.damqt* that will be read by the remaining modules. Figure 9 shows the menu displayed when this tab is pressed.

The following options can be set:

- *Highest l in expansion*: defines the order of the multipole expansion. Highest allowed value is 25 (default is 10). Expansions of the default order yield an absolute error in the atomic contributions to the density that is estimated to be less than  $10^{-5}$  a.u., except in points close to nuclei, in which around five significant figures are expected to be correct.
- *Highest l to be displayed*: determines the highest order ( $l$ ) of atomic and molecular multipole components that will be displayed and printed in the output file. It must be less than or equal to the highest  $l$  in the expansion (default is 5).
- *Type of fit*: the usual choice corresponds to fitting the total density (default), but representations of only one-center or only two-center contributions to density in the LCAO framework can be also carried out. In case of calculations using the ZDO approximation (MOPAC), the *only one-center* option is automatically set, to keep consistency.
- *Thresholds*: threshold for considering radial factors as negligible (*Cutoff*) and for truncation of radial factors expansion in Chebyshev polynomials (*Fitting*).
- *Input only*: generates the input file with the options selected. No partition or fit is actually done.
- *Parallel computing*: for systems with *mpi* installed, parallel versions of DAMSTO and DAMGTO can be run. The number of processors can be chosen and must be lower than or equal to the number of atoms in the system. This option will remain hidden for systems where *mpi* is not available or in MS-Windows systems. This option is not suitable for running *mpi* batch processes.

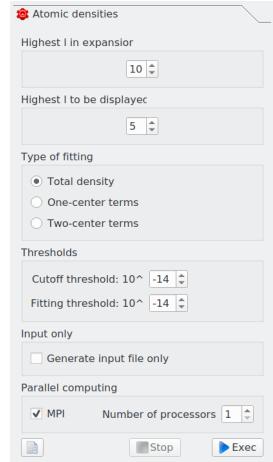


Figure 9: Atomic densities menu

The key must be pressed to compute the expansion. Besides the *\_2016.damqt*, a file, whose name ends in *\_2016.dmqtv* and which contains auxiliary integrals for electrostatic potential computation, will be created. Furthermore, some information will be displayed in the standard output (see fig 10). This information includes the project name, geometry, basis set size, total electron charge retrieved from the density (without partition), nonvanishing atomic multipole moments up to the highest order chosen for printing, and molecular charge and multipoles computed from partition. Notice that, in general, the multipole order will be lower for printing than for density fitting and computations, i.e. only a subset of the actually computed and stored multipoles will be printed. This information is also stored in a file

named *projectname*-DAMGTO320.out for GTO densities, where *projectname* stands for the name of the current project. In case of STO densities, DAMGTO will be replaced by DAMSTO.

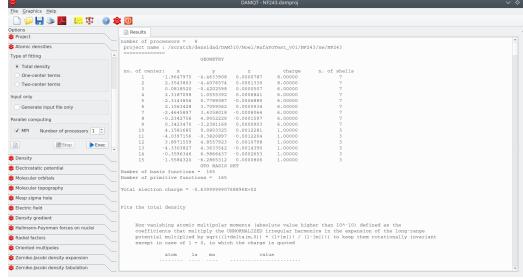


Figure 10: Standard output

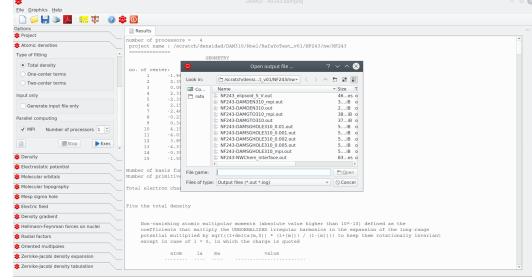


Figure 11: Standard output files menu

Another file with extension *.mltmod* containing the moduli of the atomic multipole moments is also generated. The multipole moments are defined as the coefficients that multiply the *unnormalized* irregular spherical harmonics in the expansion of the long-range potential. Since the moduli of the spherical harmonics depend on the value of  $|m|$ , the values actually stored in file *.mltmod* will be the multipole moments thus defined,  $Q_{lm}$ , each multiplied by  $(1 + \delta_{m0}) \sqrt{(l + |m|)! / (l - |m|)!}$  to keep invariance under rotations.

Key enables to stop the process. Key displays a list of all the currently available *.out* files (see

fig 11). The content of these files can be visualized in the main panel.

## 2.3 Density

*Density* tab gives access to the module for the tabulation of density and grid generation for 2D contour plots and 3D images (see fig 12). This module can deal with the density as supplied by any standard package for molecular calculations (*Original density*), i.e. expressed in terms of the basis set, or with the atomic expansion of the density generated by DAM (*Fitted density*).

When the *Original density* is selected, tabulation and grid generation can be made only for the full molecular density. The *Fitted density* option (default) opens more possibilities. Three options for density are available: *Full electron density* using an expansion starting on  $l = 0$  and ending at a user-selected  $l_{max}$  (lower than or equal to the highest available), *Density deformations* with an expansion starting in  $l = 1$  (i.e. in which the atomic spherical terms have been removed), and *Contributions to density* corresponding to a user-selected range of values of  $l$ . In each case, the multipole terms to be included in the atomic expansions can be set with the spinboxes under the label *Atomic terms*, with the pertaining restrictions. Results attained with the *Full electron density* will be similar to those of the *Original density* option but replacing the original density by its atomic multipole expansion up to the desired order. When the *Highest l* is equal to or higher than 5, the plots obtained in both ways will be indistinguishable.

Choosing *Density deformations*, the bond skeleton of the molecules and some of their patterns can be visualized and related with several concepts of the empirical structural chemistry such as lone pairs, single, double, triple bonds, electron delocalization and so forth.

To get smooth 3D surfaces in not very big systems, it is recommended to check the *gradient* box so that grids with the gradient components are computed analytically. This approximately doubles the computational time with respect to the computation of density alone. Details on how to get smooth surfaces in big systems can be found in section 4.13.10.

Furthermore, using the atomic expansion, atomic contributions to density or atomic deformations can be obtained for single atoms or groups of atoms (functional groups). Checking the box labeled *Atomic fragments*, a table is displayed to select the atoms whose densities or deformations are to be individually tabulated (see fig 13). Checking the box labeled *Functional group*, the density or deformations are tabulated for the selected atoms altogether. Indices of centers can be supplied in the box, either separated by commas or as ranges specified with the starting and ending indices separated by a hyphen.

The *Grid* options determine whether a grid for 2D plots or 3D image of density or deformations will be generated or not.

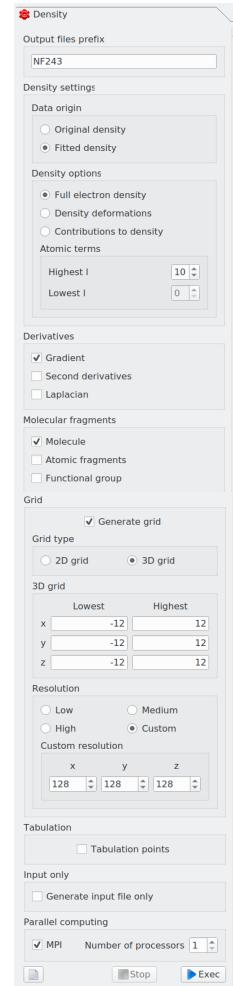


Figure 12: Density menu

If the *Generate grid* box is checked (default), and the 2D grid option selected, a panel like that shown in fig 14 is opened for tabulation settings. 2D grids are defined in terms of two variables  $u$  and  $v$  whose tabulation ranges are supplied in the boxes under the labels *Lowest* and *Highest*.

Option *Plane* carries out tabulation on a plane. Buttons are available to choose  $XY$ ,  $XZ$ ,  $YZ$  or arbitrary planes. Arbitrary plane parameters can be supplied in the suitable boxes which appear when button labeled *Other* is checked.

Checking option *Parametric surface*, tabulation is carried out for a set of space coordinates  $x$ ,  $y$ ,  $z$  computed as functions of  $u$  and  $v$ :  $x(u, v)$ ,  $y(u, v)$ ,  $z(u, v)$ . Usual arithmetic operators:  $+$ ,  $-$ ,  $*$ ,  $/$ ,  $\wedge$ , as well as the functions sin, cos, tan, log, ln, abs, exp, sqrt, can be used to define  $x$ ,  $y$ ,  $z$ . In this way, a high flexibility in the choice of 2D surfaces is provided. Three standard resolution levels can be chosen: *Low* (129x129), *Medium* (257x257), or *High* (513x513). Alternatively, user-supplied resolution can be set pressing the *Custom* button, in which case a set of spin-boxes will appear to set the resolution in both dimensions. Numbers introduced in these boxes fix the number of voxels in each direction (i.e. the number of points minus one). 2D grid tabulated values are stored in a file with a name starting with the label set in the *Output file prefix* option and with extension *.cnt*. Parallel version of the program is not allowed for 2D grids tabulation.

If the 3D grid option is chosen (see fig 15), the grid will consist of a box with the dimensions of  $x$ ,  $y$  and  $z$  coordinates supplied in the corresponding boxes under the labels *Lowest* and *Highest*, and with the chosen resolution: *Low* (65x65x65), *Medium* (129x129x129), or *High* (257x257x257). User-supplied resolution is also available. Grid tabulations are stored in files with a name starting with the label set in the *Output file prefix* option and with extension *.plt*. These files are compatible with other packages for 3D plotting such as gOpenMol<sup>5</sup>. For systems with *mpi* installed, parallel computing can be chosen as in case of *Atomic densities*.

To distinguish the different grid files generated (and from those corresponding to electrostatic potentials) the following naming conventions hold:

*\$fname-d.cnt*: 2D grid tabulation file for the full molecular density or deformations.

*\$fname-d-d?.cnt*: 2D grid tabulation files with first derivatives (? :  $x, y, z$ ).

*\$fname-d-d???.cnt*: 2D grid tabulation files with second derivatives (?? :  $xx, xy, ...zz$ ).

*\$fname-d-lplc.cnt*: 2D grid tabulation files with the Laplacian of the atomic density or deformation.

*\$fname-d.plt*: 3D grid tabulation file for the full molecular density or selected contributions to density.

*\$fname-deform-d.plt*: 3D grid tabulation file for the full molecular density deformations.

*\$fname-cxx-d.plt*: 3D grid tabulation file for the atomic density of  $xx^{th}$  center according to the ordering established in the geometry definition.

*\$fname-deform-cxx-d.plt*: 3D grid tabulation file for the atomic density deformation of  $xx^{th}$  center according to the ordering established in the geometry definition.

*\$fname-frg-d.plt*: 3D grid tabulation file for the density of selected atoms altogether (functional group).

*\$fname-frg-deform-d.plt*: 3D grid tabulation file for the density deformation of selected atoms altogether.

*\$fname-\*d-d?.pltd*: 3D grid tabulation files with first derivatives of density or deformations (? :  $x, y, z$ ).

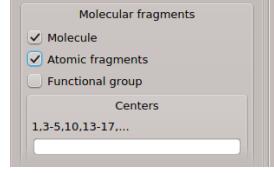


Figure 13: Single atom densities

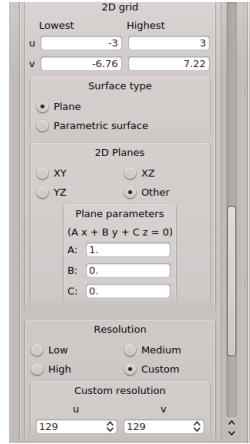


Figure 14: 2D Grid settings

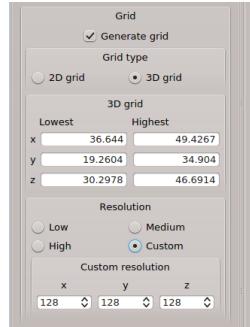


Figure 15: 3D Grid settings

`$fname-*-d-d??.plt`: 3D grid tabulation files with second derivatives of density or deformations (??  
 $xx, xy, ...zz$ ).

`$fname-*-d-lplc.plt`: 3D grid tabulation files with the Laplacian of the atomic density or deformations.  
`$fname` stands for the root name.

Besides grid generation, molecular density or its deformations can be tabulated in selected points. This can be done checking the box *Tabulation points* and specifying the points in the table. In this case, the tabulated values will be printed in the corresponding `.out` file and displayed in the main panel.

Options for input file generation and parallel computation are also available like in case of density partition and fit.

## 2.4 Electrostatic potential

Tab *Electrostatic potential* invokes the module for the tabulation of the electrostatic potential and grid generation for 3D images (see fig 16). Electrostatic potential is computed using the density representation. The number of terms included in the expansion is set with the spinbox labeled *Highest l in expansion*.

Computation using point atomic multipoles can be done checking the box labeled *Long-range only*; otherwise, a threshold for long-range is set: the contribution of an atom to the electrostatic potential in a given point will be computed from the long-range expansion only if the estimated contribution of the short-range terms is smaller than the threshold; if it is larger, the radial factors (depending on  $r$ ) will be used.

For 2D and 3D grid definitions the same comments as in *Density* hold, as well as the same resolution options. In particular, to get smooth 3D surfaces in not very big systems, check the *gradient* box so that grids with the gradient components are computed analytically. This approximately doubles the computational time with respect to the computation of electrostatic potential alone. For smooth surfaces in big systems see section 4.13.10.

For systems with *mpi* installed, parallel computing can be chosen as in case of *Atomic densities*.

File names follow a convention analogous to that mentioned in case of density. Thus, grid files are named `$fname-p.plt`, files with first derivatives of the potentials are named `$fname-p-d?.plt`, and so forth. Root name `$fname` can be set in the *Output file prefix* box. These files are also compatible with gOpenMol.

Options for input file generation and parallel computation are also available.

## 2.5 Molecular orbitals

Tab *Molecular orbitals* creates 2D and 3D grids for plotting molecular orbitals (fig 17). For options and grid definitions, same comments as in sections 2.3 and 2.4 hold. Indices of molecular orbitals to be plotted are given, separated by commas, in the box labeled *Molecular orbitals*. Ranges of indices can be defined using hyphens as separators.

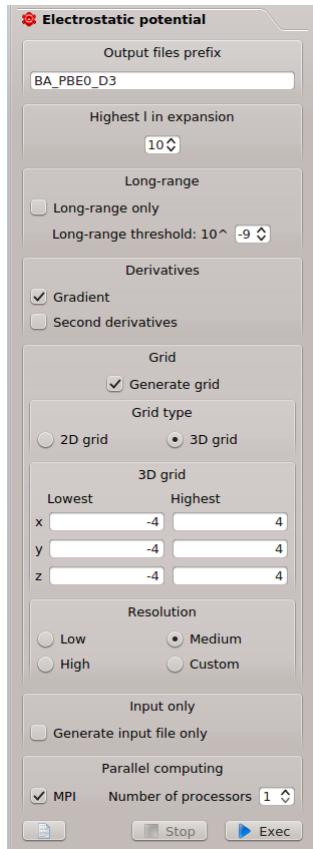


Figure 16: Electrostatic potential

<sup>5</sup>[www.csc.fi/gopenmol/](http://www.csc.fi/gopenmol/)

Molecular orbitals are sorted on ascending energy. In case of UHF calculations with MOLPRO, different sets of orbitals are obtained depending on the interface used. See section 5.2 for details.

## 2.6 Molecular topography

Tab *Molecular topography* is intended for mapping of critical points (CPs), determination of molecular graph and computation of atomic basin borders for both electron density and electrostatic potential (fig 18). Mapping of all the critical points is the first step required for any further calculation *viz.* determination of molecular graph and atomic basins.

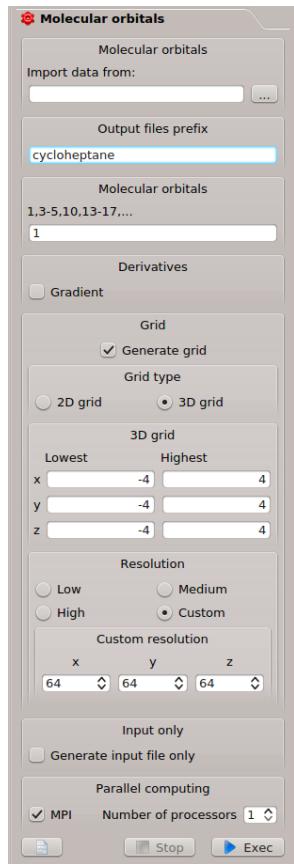


Figure 17: Molecular orbitals

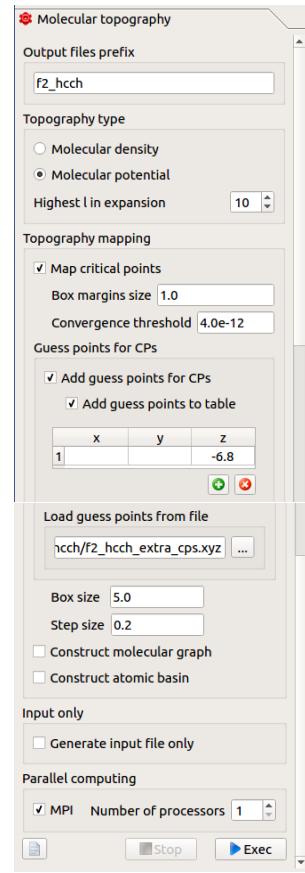


Figure 18: Molecular topography

The values of density (MED) and electrostatic potential (MESP), their gradient and second derivatives are calculated while finding the CPs using DAM partition/expansion method. The number of terms included in the expansion for calculation of field values can be set with the spinbox labeled *Highest l in expansion*. The guess points required for initiating the search of critical points are determined internally. However, especially in case of electrostatic potential, where CPs can be located far from molecular skeleton, guess point generation requires gradient evaluation on a grid. The size of the grid and step-size can be altered under the option *Guess points* by mentioning the optimal *Box size* and *Step size* in atomic units. User may intuitively provide additional guess points, if required, by checking *Add guess points for CPs*. The points can be supplied in a pop-up table or, alternatively, in an external text file, whose record must contain values of (*x*, *y*, *z*) coordinates of the points (one point per line).

These guess points are optimized to critical points using L-BFGS subroutine, an iterative method for solving unconstrained nonlinear optimization problems. The search of a critical point starting from the guess point is performed within a cubical region around latter. A cube of side ranging  $0.5 - 1.0$  a.u. is recommended for this purpose. The control over the size of this cube is provided under the option *Box margins size* which appears on checking the *map critical points* option. A convergence threshold is required for determining if the program has reached the critical point. It is optimal to provide lower value of threshold for electron density than electrostatic potential *e.g.*  $4 \cdot 10^{-16}$  and  $4 \cdot 10^{-12}$  respectively. Molecular graph for MED and MESP-based topograph is calculated using the option *Gradient path*. This primarily requires the file containing the critical points to start the calculation. Absence of CP file will automatically instruct to perform the mapping of critical points. The gradient paths leading to asymptote requires to be bound by a large box of recommended side length of 5.0 a.u.

Atomic basins for MED and MESP are calculated under the option *Atomic basin*. This computation requires the file containing the CPs and the determination of molecular graph. Checking the *compute basin* option, automatically checks the option of *gradient path*. The appearance of the basin can be corrected by checking the *Extra connections* box, and setting the *Connection threshold* value. The greater the value, the higher the number of connecting lines appearing in the basin.

The files containing critical point are named *\$fname-cps-d.xyz* and *\$fname-cps-v.xyz*, depending on whether they store MED CPs or MESP CPs respectively. Corresponding files with name *\$fname-cps-d.eigv* or *\$fname-cps-v.eigv* contain eigenvector information in the same order of CPs mentioned in the file containing CPs. The files containing molecular graph information are stored in *\$fname-d.gpdata* or *\$fname-v.gpdata*. In case of atomic basins, the surfaces are stored in *\$fname-d.basins* or *\$fname-v.basins*.

Options for input file generation and parallel computation are also available.

## 2.7 MESP sigma hole

Tab *MESP sigma hole* handles the module for the computation of molecular electrostatic potential (MESP) on an isosurface of density (MED) (fig 19). The values of MESP at the vertices of the triangles in which the MED isosurface is decomposed are stored in a file with extension *.sgh*. Furthermore local maxima (minima) higher (lower) than a given threshold are searched. The threshold is set as a fraction of the absolute extrema values in the box labeled *Threshold for local extrema*. The default value is 0.90 (90% of the absolute extrema values). A histogram of MESP on the surface (area vs MESP values) is also computed. The histogram is a plot of the surface area (in bohr<sup>2</sup>) vs the MESP value, and can be used as a tool for comparing *sigma holes* of different molecules.

To compute the sigma hole, the MED must be previously tabulated on a 3D grid (see sec 2.3), and the pertaining *.plt* file must be chosen in the box labeled as *Import density grid from*. The MED value for isosurface can be set in the box labeled as *Density value*. Three thresholds can be set in the corresponding boxes: for geometry (two points are considered the same if they are separated a distance lower than this threshold), for MESP long-range (short-range contributions are not computed when they are lower than it), and for local extrema. MESP can be computed from the DAM expansion of density (preferable) or, checking the box labeled as *Exact potential*, directly from density matrix and basis set without using the DAM expansion. Computation of exact potential is very much slower than computation from DAM

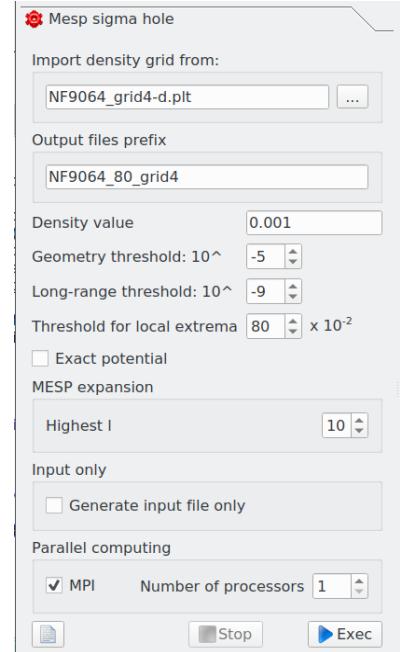


Figure 19: MESP sigma hole

expansion, and is only recommended for testing purposes.

A spectrogram of the MESP on the surface and the local extrema can be displayed with the 3D viewer included in the suite –see sec 4.13.7– and the histogram can be displayed with the built-in 2D plotter –see sec 3.3.

The program also provides statistics on MESP: average values (positive, negative and total MESP), variances, mean deviation and  $\nu$  parameter, introduced by P. Politzer, J.S. Murray et al.<sup>6</sup>

Main results of MESP statistics are collected in a file with a name appended with `_SGMESP_summary.txt`, whose content is described in appendix E.

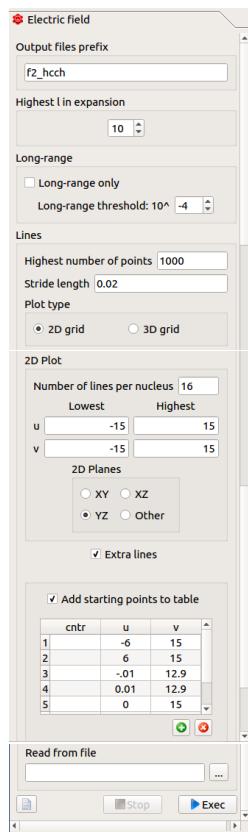


Figure 20: Electric field

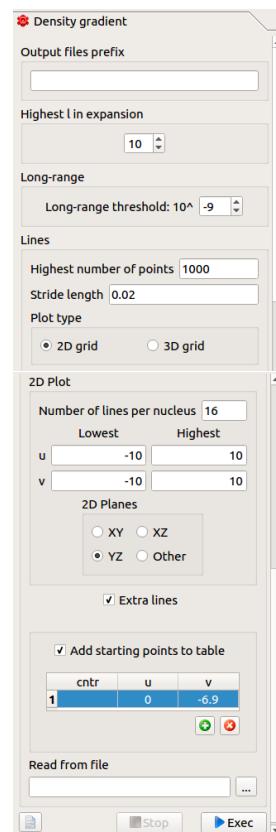


Figure 21: Density gradient

## 2.8 Electric field

Tab *Electric field* manages the module for the computation of electric field lines from the atomic multipole expansion (fig 20). The computation is made in points separated by user-supplied steps along each selected line. This module also computes 2D atomic basins of electrostatic potential in molecular symmetry planes, provided that the critical points of electrostatic potential have been previously computed in the *Molecular topography* module.

Boxes labeled *Highest number of lines* and *Highest number of points* are used to set the maximum number of lines and points per line to be evaluated, and step size is set in the box labeled *Stride length*. The size of the space region in which lines will be computed is defined in the same way as employed for defining

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<sup>6</sup>P.P. Politzer, P. Lane, J.S. Murray and T. Brink, J.. Phys Chem., 96, 7938 (1992); J.S. Murray, P. Lane, T. Brink and P. Politzer, *ibid*, 97, 5144 (1993)

the 3D grid dimensions in the *Density* and *Electric field* modules. The *Set of starting directions* of lines can be chosen among the following choices, all of them based on icosahedron vertices and symmetry axes: (0) no automatic direction, (1): vertices (12 directions per nucleus), (2): C3 axes (20), (3): C2 axes (30), (4): vertices + C3 (32), (5) vertices + C2 (42), (6) C3 + C2 (50), and (7): vertices + C3 + C2 (62).

In 2D grids, the option for set of starting directions is replaced by the *Number of lines per nucleus*.

When the box *Extra lines* is checked, additional directions can be given in a pop-up table built in the GUI or read from an external file both in 3D and 2D grids. Checking the box labeled *Add starting points to table* triggers the pop-up table display, and the external text file can be specified in the box labeled *Read file from*. In 3D grids, this file must contain one record per line to be plotted with the starting point of the line specified as (free format):

ICEN      X      Y      Z

where ICEN is an integer with the index of the nucleus from which the line departs. A negative or zero value means a line starting from a point that is not a nucleus.

X, Y and Z are real numbers whose meaning depends on whether the line departs from a nucleus or not. For a line starting at a nucleus, they define the departure direction of the line. For a line which does not start in a nucleus, they just define the starting point of the line.

In 2D grids, the format is:

ICEN      U      V

with the same meaning of ICEN as before, and where U and V are the corresponding 2D coordinates. Selection of zero lines per nucleus is allowed to generate 2D basins without field lines for further 2D plotting.

## 2.9 Density gradient

Tab *Density gradient* handles the module for the computation of density gradient lines from the atomic multipole expansion (fig 21). The computation is made in points separated by user-supplied steps along each selected line. This module also computes 2D atomic basins of electron density in molecular symmetry planes provided that the critical points of electron density have been previously computed in the *Molecular topography* module.

Same comments as in electric field section hold in this case too for options and for 2D borders of basins.

## 2.10 Hellmann-Feynman forces on nuclei

Tab *H-F forces on nuclei* invokes the module for the computation of the Hellmann-Feynman forces on the nuclei of the molecule (fig 22).

DAM partition of the density facilitates a decomposition of the total HF force on a nucleus into internal and external contributions. The former correspond to the force exerted on the nucleus of a given atom by its own electron cloud, and the latter to the force exerted by the nuclei and clouds of the remaining atoms.

Notice that for a molecule in the equilibrium geometry, total forces on nuclei must be zero *provided that the wavefunction fulfills the conditions for the Hellmann-Feynman theorem to be applicable (Berlin's conditions<sup>7</sup>)*. Wavefunctions which do not fulfill the theorem yield spurious force contributions due to the lack of fulfillment. In particular, nonphysical components leading to translation and rotation of the molecule as a whole (*perpetuum mobile*) may appear.

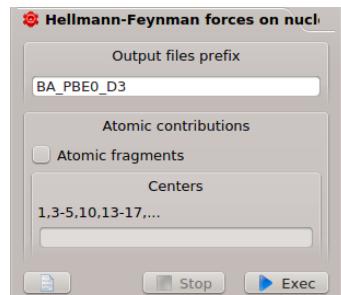


Figure 22: H-F forces

<sup>7</sup>Berlin T J Chem Phys 19 (1951) 208

DAMQT enables filtering of these spurious components by decomposing the total forces into *conformational forces* (physically meaningful), and *nonconformational forces* (physically meaningless). The latter terms may be used as a hint on the degree of fulfillment of the HF theorem by the wavefunction, in the sense that high spurious forces imply a low degree of fulfillment.

However, low spurious forces do not necessarily imply a high degree of fulfillment; in this case the degree of fulfillment should be established by other procedures. Forces are stored in a file with extension *.forces*. Besides these files, detailed information about the electrostatic potential, electric field and forces on the nuclei is given in the standard output (main panel) and stored in a file with the name ended in DAMFORCES320.out.

If the *Atoms* option is checked, individual atoms can be selected (see fig 22) for a more detailed information about the forces acting on their nuclei. In particular, the contributions of every atom to the external forces on the selected nuclei are given.

## 2.11 Radial factors

Tab *Radial factors* handles the module for tabulating the radial factors selected (fig 23). Tabulation points  $r$  are defined in an interval with user-defined starting and ending points and separated by the selected step. Further individual values of  $r$  can be added to the set by checking the box *Extra values*. A table will open where these values can be included.

Centers whose radial factors will be tabulated can be entered in the bottom box. Indices of individual centers must be separated by commas, and indices ranges can be defined with hyphens. First and second derivatives of radial factors can be also computed by checking the respective boxes.

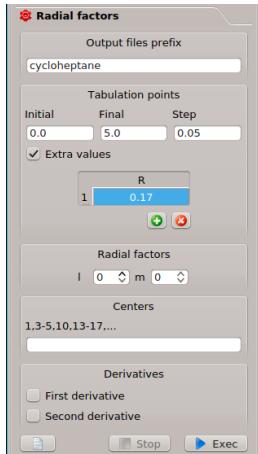


Figure 23: Radial factors

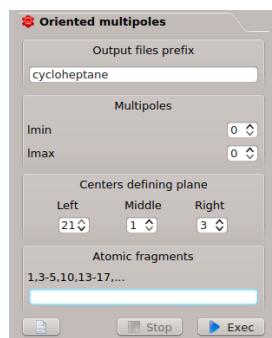


Figure 24: Oriented multipoles menu

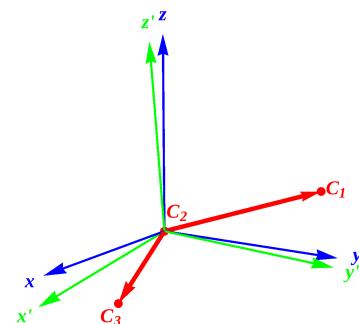


Figure 25: Oriented multipoles frame

## 2.12 Oriented multipoles

Tab *Oriented multipoles* invokes the module for locally reoriented multipoles (fig 24). These reoriented multipoles can be useful to quantify charge delocalization over a set of atoms. The atomic multipole components of density of a given group of atoms are rotated from the molecular frame, with  $x$ ,  $y$  and  $z$  axes, to a new frame whose  $z'$  axis is perpendicular to the plane defined by three selected atoms, ( $C_1, C_2, C_3$ ), and the new  $y'$  axis lies in the bisector of the angle  $\widehat{C_1C_2C_3}$  (see fig 25).

## 2.13 One-center MED expansions in Zernike-Canterakis or Jacobi functions

Tab *Zernike-Jacobi expansion* computes a one-center expansion of MED inside a ball centered at the positive charges center of the system in terms of Zernike-Canterakis or Jacobi functions (see fig 26). The expansion coefficients,  $\Omega_{kl}^m$  can be used to build rotationally invariant fingerprints,  $F_{kl}$ , of MED:

$$F_{kl} = \sqrt{\sum_{m=-l}^l (\Omega_{kl}^m)^2}$$

which can be used for molecular pattern-recognition. The coefficients  $\Omega_{kl}^m$  are stored in files with extension *.zernike* or *.jacobi* depending on the type of expansion. The fingerprints  $F_{kl}$  are printed in the output file.

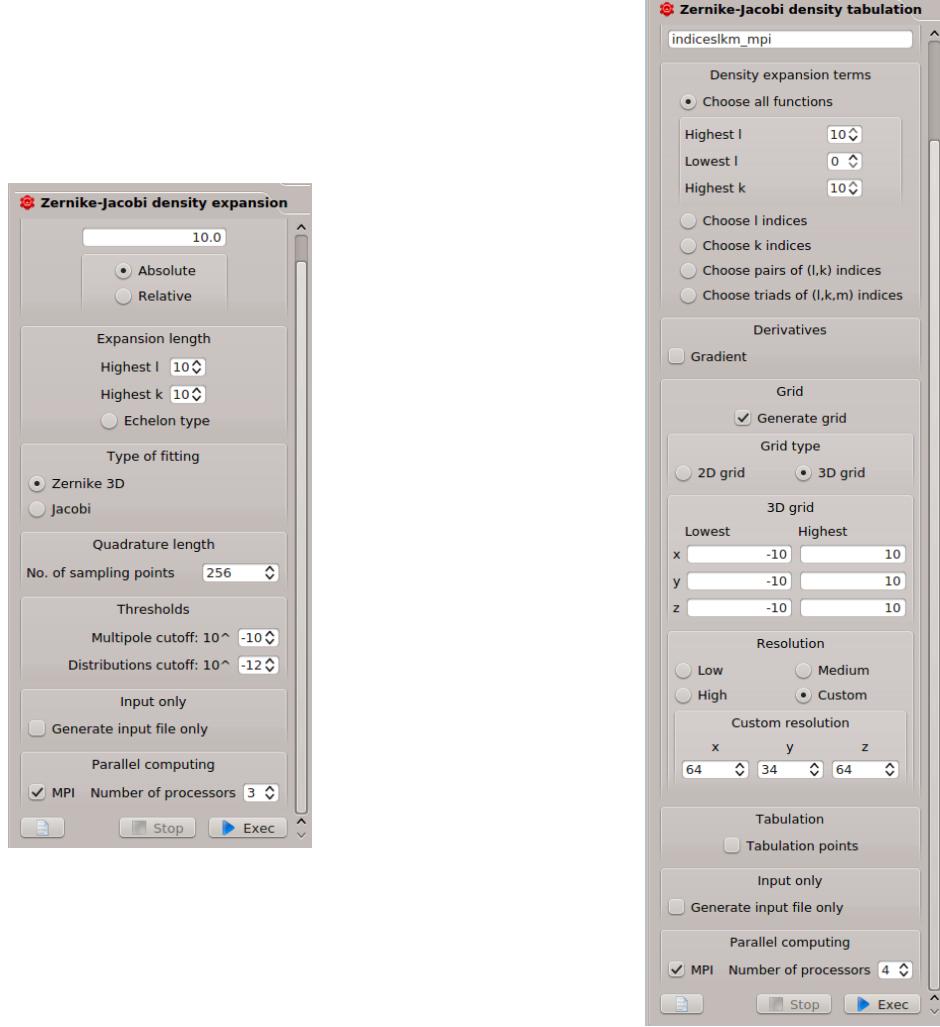


Figure 26: Zernike-Jacobi expansion

Figure 27: Zernike-Jacobi tabulation

The ball radius, and expansion type and length can be set by the user, as well as cutoffs for displaying

multipoles and neglecting charge densities in the expansion. The ball radius can be supplied as an absolute value or as an increase over the distance of the farthest nucleus to the ball center. In this case, the *Relative* button must be checked. The expansion lenght involves two indices: the  $l$  index corresponding to the spherical harmonics taken in the expansion, and the  $k$  index labeling the functions for each  $l$ . The boundaries of these indices can be taken as independent from each other (default), or in an echelon form:  $k_{top}(l) = k_{max} - l$ , if the pertaining button is checked.

As the translation techniques implemented involve a one-dimension numerical integration (quadrature) in the variable  $r$ , the size of this quadrature can be set by user.

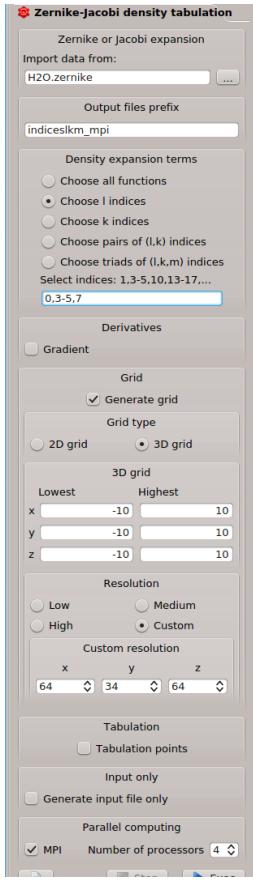


Figure 28: Choose  $l$  option

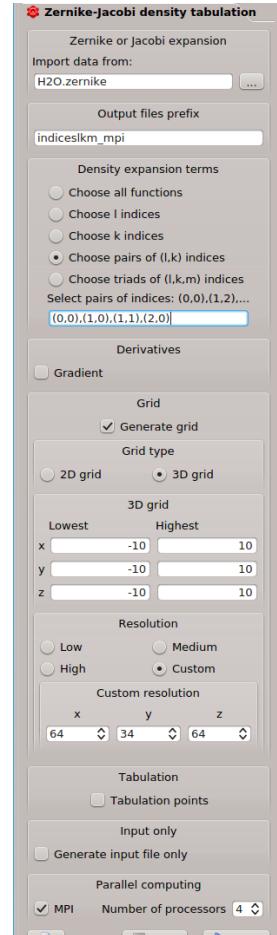


Figure 29: Choose  $(l,k)$  option

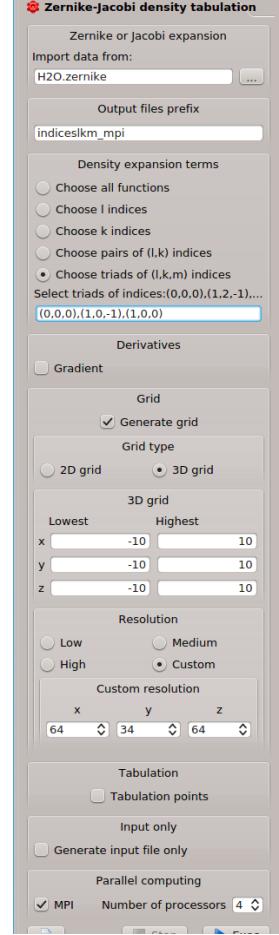


Figure 30: Choose  $(l,k,m)$  option

## 2.14 Zernike-Jacobi density tabulation

*Zernike-Jacobi density tabulation* tab gives access to the module for the tabulation of density computed with Zernike-Canterakis or Jacobi expansions inside a ball. Grids of the density thus computed can be generated for 2D contour plots and 3D images (see fig 27) that can be visualized in the 2D plotter and the 3D viewer.

Indices for projection can be selected in different ways. When the option *Choose all functions* is selected, all the functions available for projection can be chosen in the selected ranges of  $l$  and  $k$  indices, fixed

in the pertaining spin boxes. Alternatively, option *Choose l index* selects individual values or ranges of  $l$  index, with all values of  $k$  and  $m$  indices compatible (see fig 28). Commas are used as separation character and hyphens are used for ranges. Option *Choose k index* is likewise but for  $k$  index. Finally, individual pairs of  $(l, k)$  values (with all  $m$  compatible) and triads of  $(l, k, m)$  can be selected in the last two options (see figs 28 and 30). In these cases, parenthesis are just optional cosmetic aids to help in identifying pairs or triads, but are removed when generating input files.

### 3 The Graphical User Interface II: 2D Plots

DAMQT has its own 2D plotter built in the GUI. The plotter can be launched by either pressing the key  in the toolbar, by choosing *Graphics* → *2D Viewer* in the upper menu or by pressing the button labeled as *New 2D plotter* on the right menu. A 2D viewer will be displayed on top of the display, as shown in fig 31.

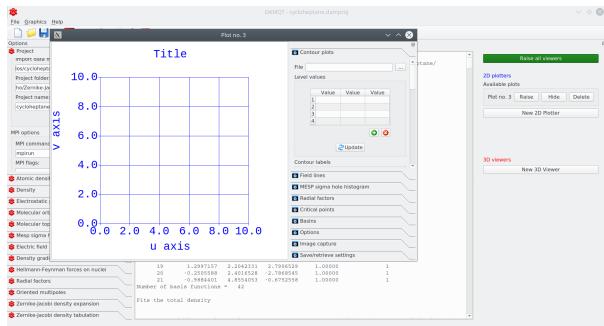


Figure 31: 2D viewer window

New 2D viewers can be launched without running any DAMQT application and several viewers can be present in one session. For each 2D viewer currently open, one key is added on the right of DAMQT main window to facilitate navigation –see fig 31.

Each 2D viewer enables plotting of contour plots of the grid tabulated MED, density deformations, MESP, molecular orbitals, electric field, density gradient, critical points and atomic basins, as well as MESP sigma hole histograms and Radial factors of atomic densities. Suitable data can be generated with the corresponding modules described in section 2 of this manual.

The 2D viewer menu consists of nine tabs labeled: *Contour plots*, *Field lines*, *MESP sigma hole histogram*, *Radial factors*, *Critical points*, *Basins*, *Options*, *Image capture*, and *Save/retrieve settings* whose contents are discussed below. The menu can be undocked by pressing with mouse left button the on the top of the menu and dragging through screen –see fig 32. Undocked menu can be also resized with the mouse and docked back by double clicking on top of the menu window or pressing key  on the upper right corner. Some operations may cause undocked menu to disappear; click on the 2D viewer to rise the menu to foreground.

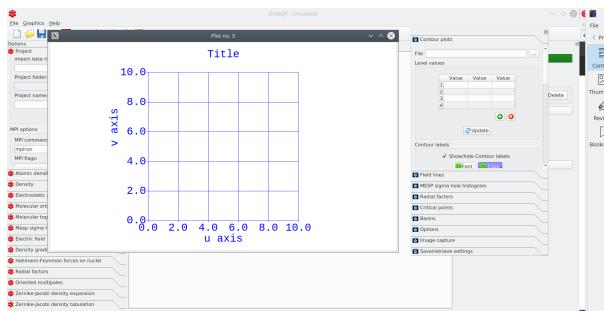


Figure 32: 2D viewer: undocked menu

Context menus are activated when suitable plots are displayed in the plotter. Inactive menus appear in light gray.

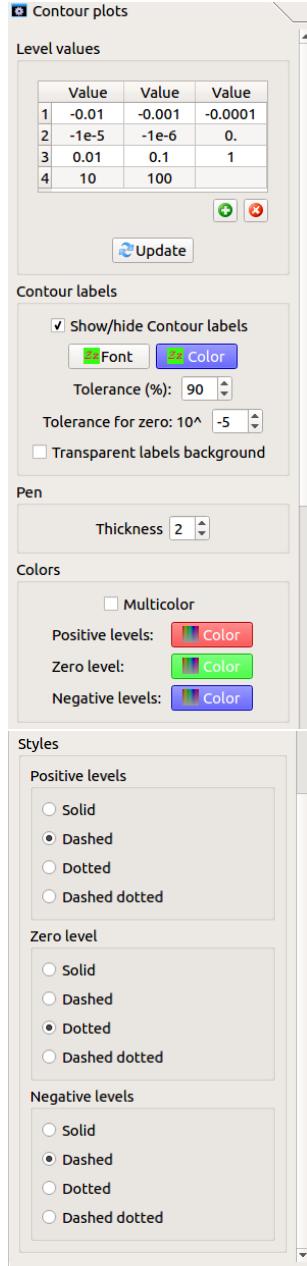


Figure 33: Contour plots

### 3.1 Contour plots

Tab *Contour plots* contains options for displaying and handling 2D contour plots (fig 33). Its content is active only when a *.cnt* file is loaded in the plotter. Level values appear in a sheet, where they can be changed, removed or added. A *tolerance* parameter is used to decide whether a clicked point is over a contour line or not. For lines lying in steep regions, it may be convenient (even necessary) to reduce the value of this parameter to facilitate labels operation. Styles for lines can be set, including thickness, colors and line types. Further options, common to other plots, can be set in the *Options* tab (see below). Contour values can be displayed over lines by double clicking on them.

Files containing grid tabulations for 2D contour plots are binary files with extension *.cnt*. Their content can be extracted to a text file with the ancillary program *readcnt.exe* also included in the package. The *readcnt.exe* also generates a file with extension *.gnu* with the tabulation in a format suitable for plotting with *gnuplot*. When tabulations refer to planes, a code is included in the name to specify the type of plane. For instance, *XY0* refers to plane *XY*, or *0YZ* to plane *YZ*.

Contours and electric field or density gradient lines can be displayed together, just loading the pertaining files and accepting that images are superimposed (see fig 34).

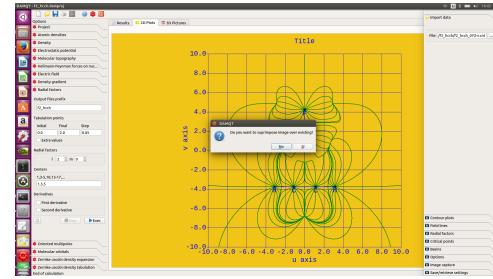


Figure 34: Combining plots

## 3.2 Field lines

Tab *Field lines* contains options for electric field and density gradient lines plotting (fig 35). Field lines can be combined with contour plots, critical points and basins. Borders of 2D basins and points corresponding to 2D critical points are searched at the same time that field lines are computed, provided the corresponding 3D critical points have been previously computed in the *Molecular topography* module. Files containing electric field and density gradient lines are text files with extensions *.cam2D* and *.dengr2D*, respectively.

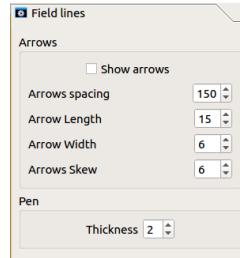


Figure 35: Field lines

## 3.3 MESP sigma holes histogram

Tab *MESP sigma holes histogram* displays options for plotting histograms with values of areas on a MED isosurface vs MESP values (fig 36).

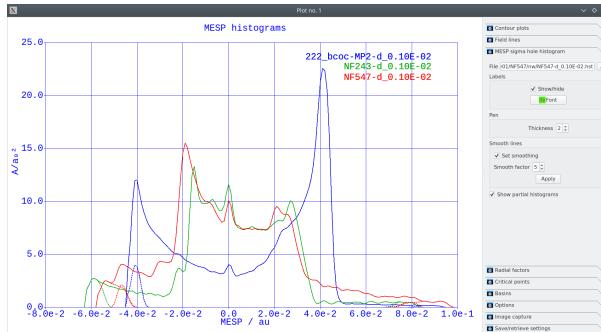


Figure 36: MESP sigma hole histogram

Checking the box labeled *Set smoothing*, histograms can be smoothed with a user supplied *smooth factor*. Each time the *Apply* button is pressed, the smoothing process is applied to the curve. Unchecking the *Set smoothing* box restores the histogram to its initial shape (without smoothing).

Several histograms can be plotted together by just loading them consecutively. When a new histogram file is selected in the upper box, the user will be prompted to decide whether the new histogram must be added to those already plotted or not (fig 37).



Figure 37: Adding curve to current plot

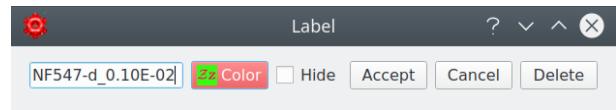


Figure 38: Histogram curve editor

When the option *Show partial histograms* is checked, the contributions of non-adjacent regions to the total histogram in the neighborhood of the extrema are also plotted (dotted line in fig 36). These partial histograms are useful to discriminate the cases in which the areas in the extrema regions correspond to a single minimum or maximum, like in the green curve of the figure, from those in which they result from the accumulation of areas associated to several minima or maxima, as in red and blue curves

Labels can be dragged by keeping the *Left* mouse button pressed on the label while displacing mouse. Double clicking on the label of a histogram opens a window for editing (fig 38). For further mouse actions see section 3.10.

### 3.4 Radial factors

Tab *Radial factors* contains options for plotting radial factors (fig 39). Its content is active only when a *.frad* file is loaded. Files containing radial factors are text files with an extension *.frad*, and those with first and second derivatives, with extensions *.drvfrad* and *.drv2frad*.

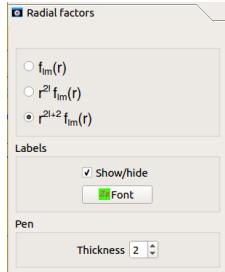


Figure 39: Radial factors

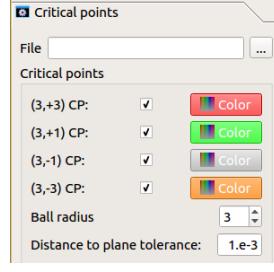


Figure 40: Critical points

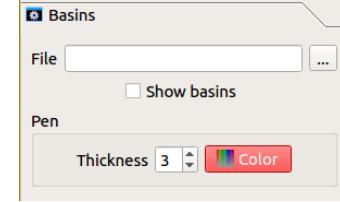


Figure 41: Atomic basins

### 3.5 Critical points

Tab *Critical points* contains options for plotting critical points (fig 40). Its content is active only when a file for contours or field lines plotting is loaded.

### 3.6 Basins

Tab *Basins* contains options for plotting atomic basins borders (fig 41). Its content is active only when a file for contours or field lines plotting is loaded.

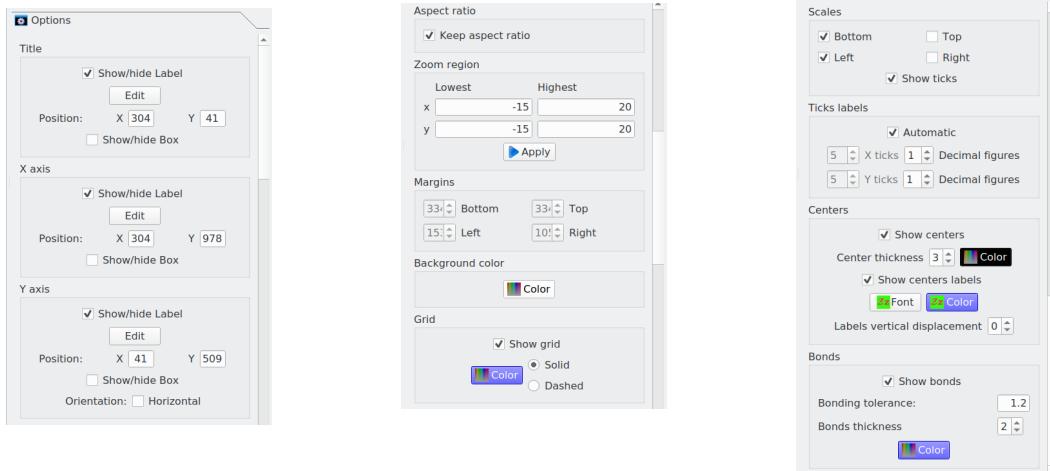


Figure 42: Options

### 3.7 Options

Tab *Options* contains general options common for all 2D plots (fig 42). Options corresponding to atom centers and bonds are active only when a file for contours or field lines plotting is loaded.

### 3.8 Image capture

Tab *Image capture* saves the plot into a file (fig 43). Several types of graphics can be chosen (*.png*, *.jpg*, *.bmp*, *.ppm*, *.tiff*, *.xbm*, *.xpm*). Resolutions up to 8192x8192 can be defined. This limit can be extended by changing definition of parameter *HIGHEST\_RESOL* in file *viewer2D.h* and recompiling.

### 3.9 Save/retrieve settings

Tab *Save/retrieve settings* is intended to save current settings to a file or to retrieve them from a previously saved *.2Dsettings* file (fig 44).

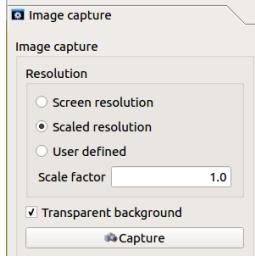


Figure 43: Image capture

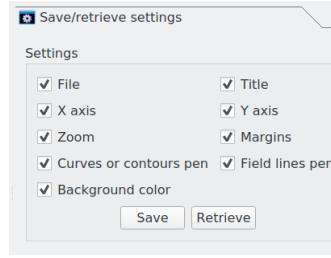


Figure 44: Save/retrieve

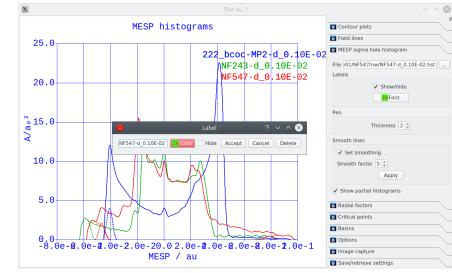


Figure 45: Sigma hole histogram popup window

### 3.10 Mouse operation

The 2D viewer supports the mouse events summarized below.

- Holding the *left button* pressed over any of the *title*, *X axis*, *Y axis*, or curve labels, labels can be displaced along the viewer.
- In contour or field lines plots, holding the *left button* pressed over atom labels, these labels can be displaced along the viewer.
- In MESP sigma hole histogram plots, curve labels can be dragged holding the *left button* pressed on them.
- Double clicking the *left button* on *title*, *X axis*, *Y axis*, or curve labels displays a window for labels editing. Changing color in curve label causes also the change of curve color.
- Double clicking the *left button* on a contour line causes the contour value to be displayed (only in contour plots).
- Double clicking the *left button* on a contour label deletes it (only in contour plots).
- Double clicking the *left button* on a curve label of MESP sigma hole histogram plots opens a window for editing the curve (fig 45).

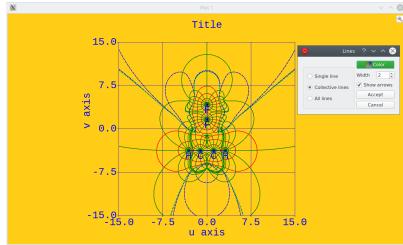


Figure 46: Field lines popup window

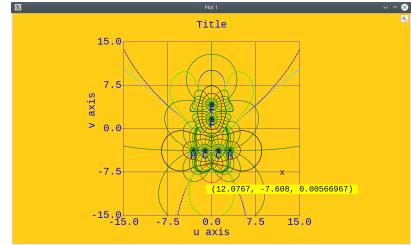


Figure 47: Point coordinates and value

- Double clicking the *left button* on a field line a pop-up menus is displayed to change colors of field lines (only in field plots). Color can be changed in a single line, a set of lines corresponding to the same basin, or all lines (fig 46).
- Holding the shift key pressed and double clicking the *left button* on a contour line, if *multicolor* option is checked, a dialog is opened for line color (only in contour plots).
- Clicking the *right button* on a point inside the plot region and out of the contour lines and labels causes the point to be displayed together with its coordinates and function value (only in contour plots) (fig 47). Click *left button* to cancel the effects of this operation.
- Holding the **Shift** key pressed together with the *left button* and moving the mouse, a rectangular region can be selected for zooming. Use keys and in the upper right corner of the viewer to navigate through zoom selections.

## 4 The Graphical User Interface III: 3D Graphics

DAMQT has also its own graphics viewer built in the GUI, which facilitates 3D plotting. The grids can be generated with some of the modules previously described in section 2 of this manual. The 3D viewer can be launched by pressing the key  in the toolbar, by choosing *Graphics → 3D Viewer* in the upper menu or pressing the button labeled *New 3D viewer* in the right menu. A new 3D viewer with menu for loading molecules data is opened (see fig 48). Several viewers can be present in the same session, each one having its own menu.

The menu contains twelve items: *Add molecule*, *Geometry measures*, *Rotations*, *Translations*, *Axes*, *Manage capture*, *Manage lights*, *Manage balls and sticks*, *Manage viewport*, *Optimize cluster*, *Save geometry* and *Save/retrieve settings*, which will be described in the following sections. The menu can be undocked and docked back in the same way as in 2D viewer.

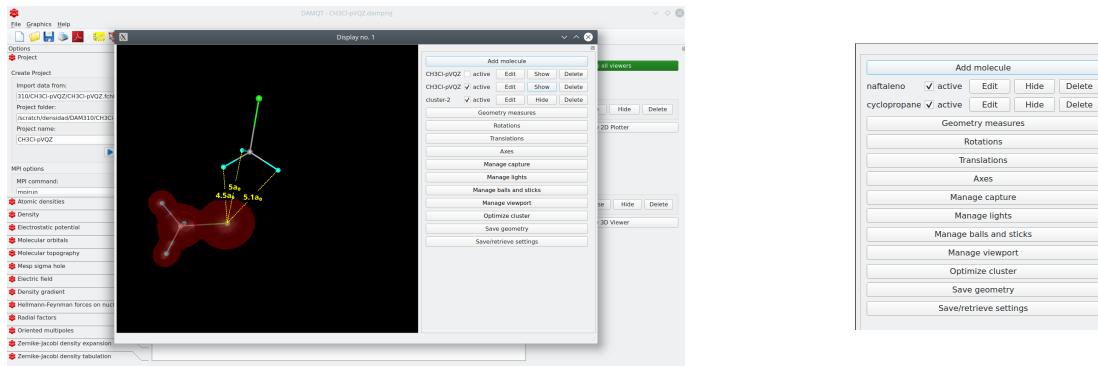


Figure 48: 3D viewer

Figure 49: 3D menu with two molecules loaded

### 4.1 Add molecule

Pressing *Add molecule* button, a window is opened to navigate through the directory tree and load a suitable file with a molecule geometry. DAMQT generated valid files are those with extensions *.ggbs*, *.sgbs* and *.xyz*. Furthermore, geometry can be loaded from any text file with the following format:

```
NCEN
a comment or blank line
ATOM1    X   Y   Z
ATOM2    X   Y   Z
...

```

where NCEN stands for the number of atoms in the molecule, ATOM $i$  stands for the atomic symbol of atom number  $i$ , and X, Y, Z are the corresponding Cartesian coordinates in Angstrom. Notice in this point that distances must be given in bohr in the *.ggbs* file, whereas they are given in Angstrom in file *.xyz*; this is so for compatibility of *.xyz* files with gOpenMol and other packages. The line after NCEN must be empty or contain a comment and it will not be processed.

To prevent misbehavior, adding molecules will not be allowed if a cluster built with the cluster optimizer is present –see section 4.10. A message will be displayed when attempting to add a molecules in these circumstances.

DAMQT carries out a change of coordinates (translation) to put the center of positive charges of the molecule at the coordinates origin, which is placed at the geometric center of the viewer.

Several molecules can be loaded into the same display, and one entry for each molecule will appear in the menu (see fig 49), containing a checkbox and three buttons for editing, hiding/showing and deleting the molecule. Pressing on the *Edit* button of a given molecule, a menu is opened for handling options corresponding to the molecule. The content of this menu will be discussed in section 4.13. If at least one molecule is active (box checked), rotation and translation operations will be performed on all active molecules (local molecular frames). When all the molecules are inactive, rotations and translations are performed on the system as a whole (laboratory frame). It is important to distinguish this behavior from that corresponding to the transformation of active molecules, specially when all the molecules in the canvas are centered at the origin. In this case, both transformations may look the same, but they are different, and careless handling of both types of transformations may cause unexpected behavior when displaying.

Activation can be toggled also by double clicking on a molecule structure while holding the **Ctrl** key pressed. When more than one molecule (either active or inactive) are placed in the same region, this only acts on the molecule loaded first. Nevertheless, molecules can be always (in)activated by checking the pertaining box in the menu.

Rotations around the *x* and *y* axes of the corresponding frame can be made by displacing the mouse while the *left button* is pressed. Vertical displacements cause rotation around screen horizontal axis (*x* axis) and horizontal displacements cause rotation around vertical screen axis (*y* axis). Rotations around *z* axis can be performed moving the mouse while keeping the *right button* pressed.

When a molecule is not active, its structure and surfaces appear darker than when it is active.

Translations can be made by keeping both the **Shift** key on the keyboard and the *left button* of the mouse pressed while displacing it. Zooming can be performed in the same way but pressing the *right button* instead of the *left button*, or using the mouse wheel.

Alternatively, translations can be carried out pressing some keys on the keyboard, according to the following scheme: **W**: zoom in; **S**: zoom out; **A**: left; **D**: right; **Q**: up; **Z**: down. Rotations can be made also by pressing some keys: **R**: rotate around screen *Y* (vertical) axis; **E**: rotate around screen *X* (horizontal) axis; **F**: rotate around screen *Z* (perpendicular) axis. Keeping *shift key* pressed the rotation is reversed.

Finally, these transformations can be made also in the corresponding menus, either those appearing in the main menu, for the laboratory frame, or those in the molecular editor –see section 4.13– for the local molecular frames.

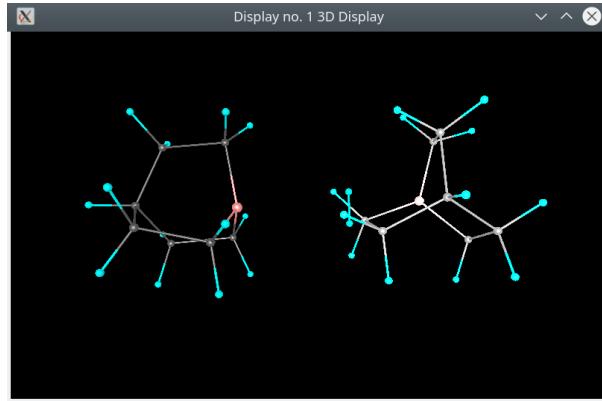


Figure 50: 3D display

## 4.2 Geometry measures

Use the *Geometry measures* button to measure distances, angles and dihedral angles between atomic centers or critical points of the molecules displayed in the canvas. Pressing it, a window appears with

four buttons to choose the type of measures –see fig 51. Each button opens a menu for the corresponding type of measures to be done and *None* button closes the measures submenus.



Figure 51: Measures window

To measure a distance between a pair of centers, the *Distances* button must be checked, and the pairs of centers are chosen by double clicking on them in the display while keeping the **Shift** key pressed. The last selection will appear in the bottom of the menu window –fig 52– and the results can be displayed in the viewer –fig 53– or in a separate window –fig 54–. A subscript indicates the molecule which contains the center (molecule index).



Figure 52: Distances menu

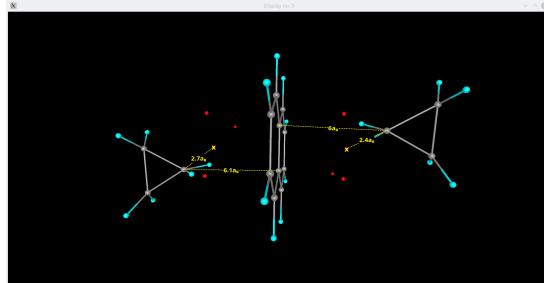


Figure 53: Distances display

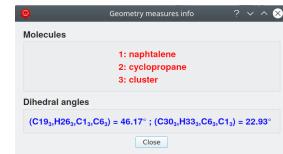


Figure 54: Distances window

To measure the angle between three centers, the *Angles* button must be checked, and the centers are chosen by double clicking on them in the display while keeping the **Shift** key pressed. The second center is that placed in the vertex. The last selection will appear in the bottom of the menu window –fig 55– and the results can be displayed in the viewer –fig 56– or in a separate window –fig 57–.



Figure 55: Angles menu

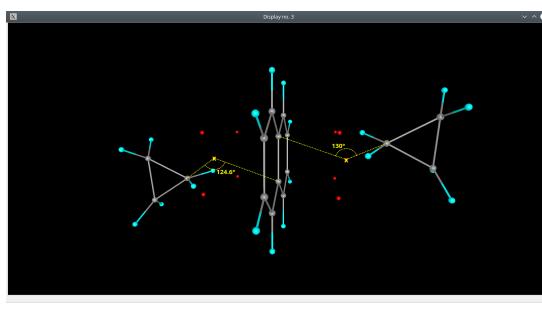


Figure 56: Angles display

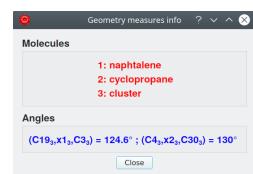


Figure 57: Angles window

To measure the dihedral angle between four centers, the *Dihedral angles* button must be checked, and

the centers are chosen in the same way as indicated for distances and angles. The first three centers define one plane and the second plane is defined by centers 2, 3, and 4. The last selection will appear in the bottom of the menu window –fig 58– and the results can be displayed in the viewer –fig 59– or in a separate window –fig 60. A subscript indicates the molecule which contains the center (molecule index).

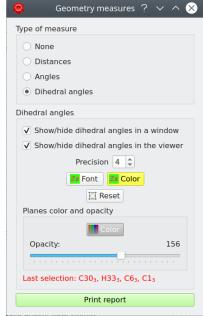


Figure 58: Dihedral angles menu

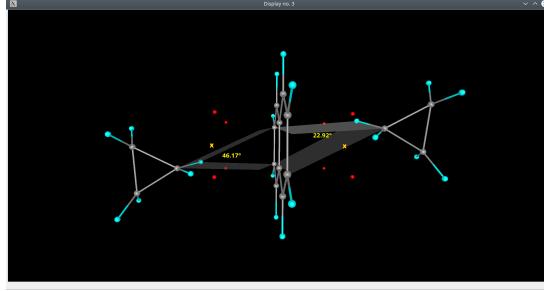


Figure 59: Dihedral angles display

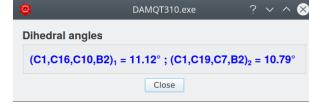


Figure 60: Dihedral angles window

To remove an angle, a dihedral or a distance, double click on its label.

### 4.3 Rotations

The *Rotations* button opens a menu for laboratory rotation manager –see fig 61. The components of the current rotation axis are displayed together with the rotation angle in degrees. Changing the boxes content and pressing *Enter* on the keyboard or clicking *Apply* button carries out the rotation specified in the boxes. This rotation is applied to the original axes, not to those currently displayed. When rotations are performed with the mouse, as mentioned in section 4.2 the boxes content is automatically updated. Rotations with respect of screen axes can be animated by checking the pertaining boxes. The *Start* (*Stop*) button toggles the animation.

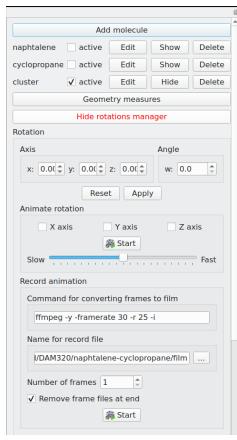


Figure 61: Rotations menu

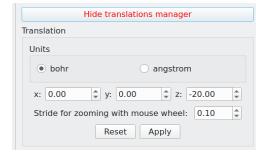


Figure 62: Translations menu

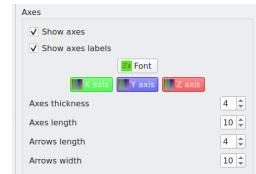


Figure 63: Laboratory axes

This feature can be combined with the *Record animation* to capture frames and making movies. Frames are individually captured in PNG files which can be optionally saved, and the set of frames is assembled into a movie in a file with mp4 format.

The file with the recorded animation is built from the single frame files with `ffmpeg`, but this can be replaced by any other suitable program. A box is supplied with the instruction to be run for recording, so that recording program and options can be set in it. The full name (including path) of the record file and the number of frames to be captured can be set in the pertaining boxes. The installation of `ffmpeg` or the alternative recording program is left to user.

A checkbox is available to determine whether the file of single frames will be removed (the default) once the movie file is built or not. A *Start* (*Stop*) button is included to control recording. In this case, animation ends when recording finishes or when the *Stop* button is pressed.

#### 4.4 Translations

The *Translations* button opens a menu for laboratory translation manager –see fig 62. The components of the translation vector are displayed in three boxes which are synchronized with the translations carried out by mouse displacements, as commented in section 4.2. Changing the content of the boxes and pressing *Enter* on the keyboard or clicking *Apply* button carries out the translation specified in the boxes. Translation values can be supplied in bohr or in angstrom, by checking the pertaining button.

#### 4.5 Axes

The *Axes* button opens a menu for displaying and customizing laboratory frame axes –see fig 63.

#### 4.6 Capture manager

The *Manage capture* button displays a menu for capturing an image of the 3D viewer content and saving it to a file –see fig 64. Images can be saved in the following formats: PNG, JPG, BMP, JPEG, PPM, XBM, XPM, TIFF. The format is specified in the file extension. High resolution can be achieved by suitable scaling.

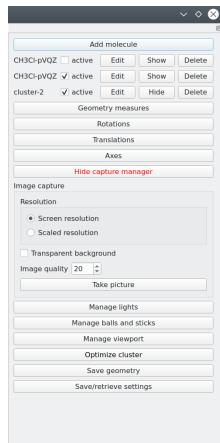


Figure 64: Image capture

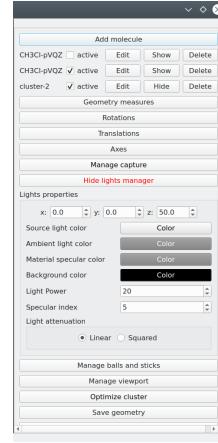


Figure 65: Lights

#### 4.7 Lights manager

The *Manage lights* button displays a menu for lighting options, including background color –see fig 65. Lighting is achieved by means of a point source placed at the point whose coordinates are displayed in the boxes, and an ambient light source. Reflection properties can be set, as well as the source light power. Press *Return* key to apply the changes in the boxes values. Attenuation can be linear or squared.

## 4.8 Balls and sticks manager

The *Manage balls and sticks* button displays a menu with options for balls and sticks used in the molecular structure display –see fig 66.

Balls and cylinders radii can be scaled by user, and threshold for bond plotting can be changed. Atoms separated by less than or equal to this threshold times the sum of their van der Waals radii will be connected with a bond stick.

## 4.9 Viewport manager

The *Manage viewport* button displays a menu with options for viewport –see fig 67– including *Far* and *Near* clipping planes.

Clipping planes can be used to get slices of 3D images –see fig 68. To do that, start by setting the *Far* plane at a suitable distance so that the surface contour corresponds to the cut, next change the *Near* plane to remove the innermost part of the surface until the desired cut is achieved. Notice that this procedure can be used also to visualize inner parts of large systems. The *Translation* menu of the *Molecule* editor –see section 4.13.4– can be helpful to choose suitable values of *z* for cut.

Once suitable cutting planes have been chosen, slices of the surface can be changed moving the plane along the *z* axis by displacing the mouse with the *Shift* key and the *right button* pressed or rolling the wheel. The slices quality is improved if the surface *Wire frame* mode is chosen –see 4.13.9.

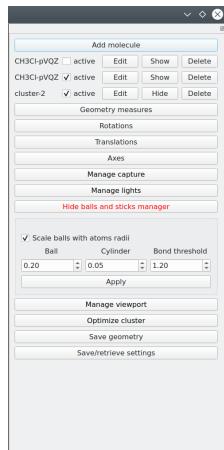


Figure 66: Balls and sticks

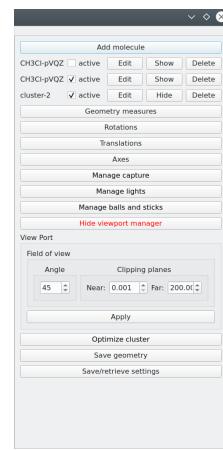


Figure 67: Viewport

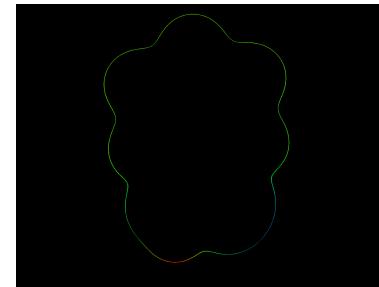
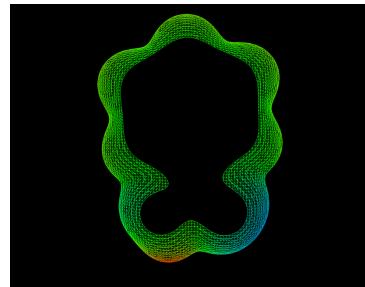
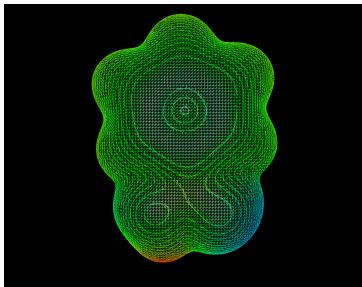


Figure 68: 3D surface slices

## 4.10 Optimize cluster

The *Optimize cluster* button displays a menu –see fig 69– with options for cluster building using the EPIC method as proposed by Gadre et al.<sup>8</sup> In this procedure clusters are generated by adding *guest* molecules to a *host* molecule. Therefore, at least only one molecule must be added to the canvas. If only one molecule is present, it will act both as host and guest, in the template mode.

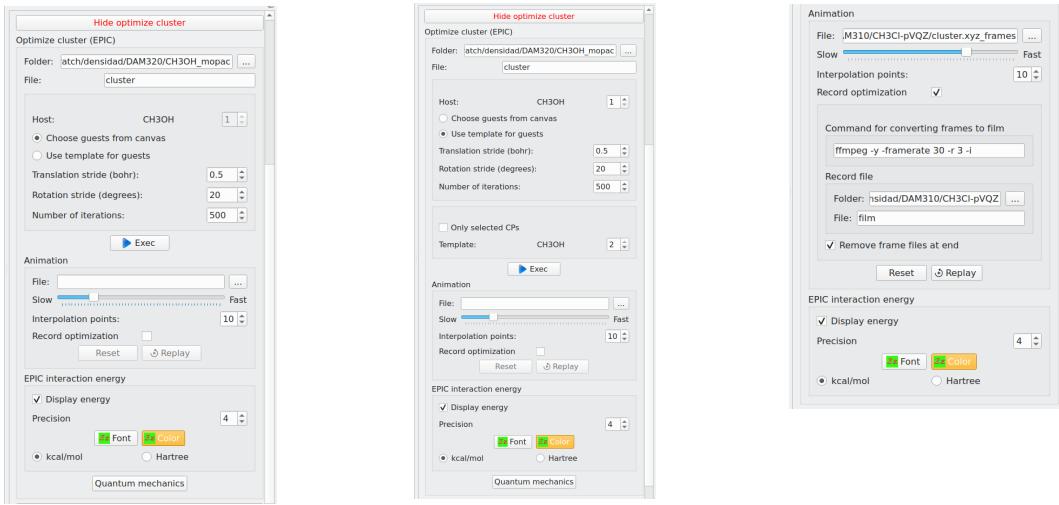


Figure 69: Cluster building: first way

Figure 70: Cluster building: second way

Figure 71: Record animation

There are two ways to build a cluster. The first one can be chosen by checking the button with the legend *Choose guests from canvas*, and requires at least two molecules loaded. The molecule loaded first will be the host, and the remaining ones will act as guests. In this way, a starting point will be prepared from the molecules as displayed in the canvas, and the user has to arrange them in appropriate positions. If the EPIC program finds that some molecules lie too close to the host, it will carry out a displacement on the implied guests to put them at a sufficiently long distance to prevent clash.

The second way is activated by checking the button with the legend *Use template for guests* –see fig 70. It uses as starting point the critical points (CP) of the host MESP. In this case, having one molecule in the canvas is sufficient, as it may act both as host and guest template. A file containing the host MESP CPs (\*.cps-v.xyz) must be loaded, and the pertaining CPs (only (3,+3)) will be used in full or in part, by selecting them as indicated in section 4.13.9. If only selected CPs are wanted as starting points, the box labeled as *Only selected CPs* must be checked. The position of the molecules is irrelevant, as it will take the host centered at lab origin and the guest molecules, at the selected CPs.

Strides for translation and rotation can be set in the respective boxes.

Pressing the button labeled as *Exec*, geometry optimization will start. During optimization, a legend reading *Computing...* will appear in the status bar (left bottom), and the changes in geometry will be reflected in the canvas. The legend will disappear once the process is completed, and a box will be displayed with a message saying that optimization has finished.

<sup>8</sup>Gadre S, Babu K Resonance 4 (1999) 40

**Important:** wait until the finalization message appears, as there is some overhead time after the optimization steps have been accomplished.

Optimization generates a file with extension *.xyz\_frames* which contains the geometries corresponding to every step. This file can be used to display an animation of the process. This can be done by loading the file in the pertaining box, and pressing the button *Replay*. Animation may include geometrical parameters as distances, angles and dihedral angles, selected as commented in section 4.2. The starting geometry can be recovered by pressing the button labeled as *Reset*.

In the animation, an interpolation between computed frames is made to smooth the movements. The animation can be recorded in a similar way as that employed for rotations by checking the box labeled as *Record optimization* and pressing the *Replay* button. Same options as in case of animating rotations –see section 4.3– are applicable.

When a cluster is present in the viewer, no further molecules can be added to it. The cluster must be the last *molecule* present in the menu, and it has to be removed to allow loading further molecules in the canvas.

In appendix F, some strategies to facilitate usage of cluster optimization are discussed.

## 4.11 Save geometry

Pressing the button *Save geometry* a window is open for saving a file with the Cartesian coordinates (in angstrom) of all molecules displayed in the canvas. First molecule is labeled as *host* and the following ones, as *guests*.

## 4.12 Save/retrieve settings

The *Save/retrieve settings* button saves the current settings of the image display or retrieves settings previously saved –see fig 72. Files with settings have extension *.3Dsettings*.

Clusters built with the optimizer tool will not be saved in the *\*.3Dsettings* file. They can be retrieved by loading the pertaining *\*.xyz\_frames* file as indicated in section 4.10.

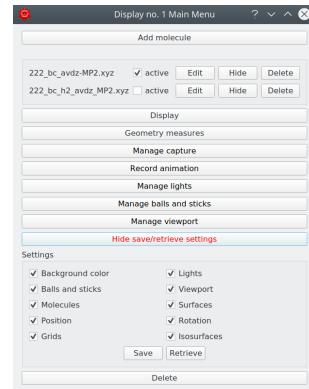


Figure 72: Save/retrieve

## 4.13 Molecule editor

As mentioned in section 4.1 when a molecule is added to the viewer, an entry will be placed in the main menu of the viewer with one checkbox to activate/deactivate the molecule for translation/rotation operations and three buttons labeled as *Edit*, *Hide* and *Delete*.

The *Hide* button will toggle between hiding and showing the structure and surfaces corresponding to the molecule. The label itself will change to *Show* when the molecule is hidden.

The *Delete* button displays a window asking for confirmation of the molecule deletion –see fig 73. Acceptation causes the corresponding molecule and all properties related to it (structure, surfaces, critical points, field lines, etc) to be removed from the viewer.

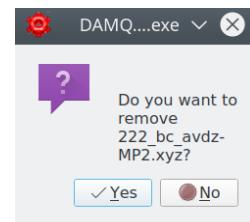


Figure 73: Delete molecule confirmation

The *Edit* button opens a window with a menu for editing the molecule as shown in fig 74. Ten options for edition appear in the menu: *Molecular skeleton*, *Labels*, *Rotations*, *Translations*, *Axes*, *Hellmann-Feynman forces*, *3D Field lines*, *Critical points*, *Add surface*, and *Add grid for isosurfaces*. Each button opens a window with a suitable menu to carry out the pertaining operations. A brief description of these options follow.

When the molecule editor window is open, pressing the *Edit* button brings the window to the foreground. This is useful in cases in which the molecule editor is hidden by some operations in the display.

#### 4.13.1 Molecular skeleton

Pressing the *Molecular skeleton* button, a menu like that shown in fig 75 is displayed in the editor to show/hide atoms, bonds or hydrogens in the structure.

#### 4.13.2 Labels

Pressing the *Labels* button, a menu for handling atom labels is displayed –see fig 76. If any of the checkboxes in the menu is marked, a new box with the option for displaying only selected centers appear that, when checked, adds new buttons for operation –see fig 77. Selection/deselection for labels display is carried out by double clicking on the required centers. Another way to toggle center selection is to double click on the display while holding the *Shift* key. In this case, a popup window appears where the center to be toggled can be chosen –see fig 78. This procedure is specially useful for big systems, in which locating a given center in the structure display can be difficult.

Furthermore, symbols font type, size and color can be changed by pressing the pertaining buttons in the menu.

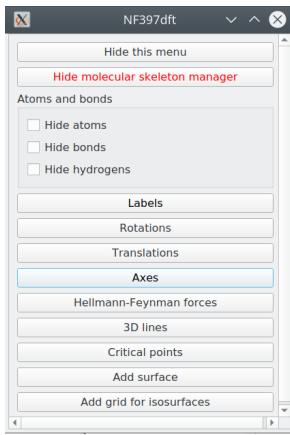


Figure 75: Molecular skeleton

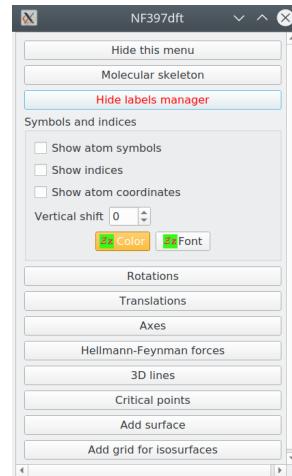


Figure 76: Atom labels

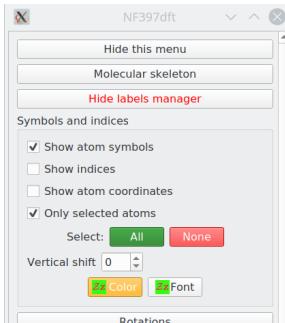


Figure 77: Select atoms

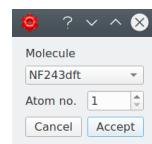


Figure 78: Selection menu

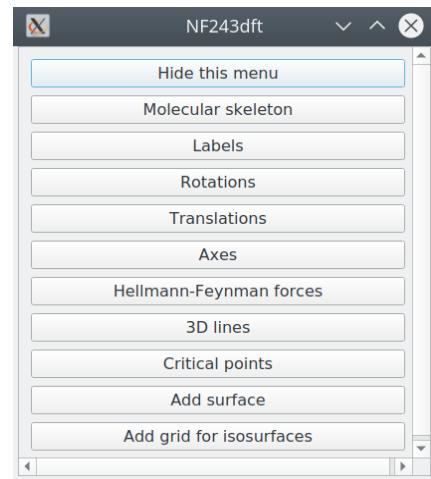


Figure 74: Molecule editor

### 4.13.3 Rotations

The *Rotations* button opens a menu for rotation manager –see fig 79. The components of the current rotation axis are displayed together with the rotation angle in degrees. Changing the boxes content and pressing *Enter* on the keyboard or clicking *Apply* button carries out the rotation specified in the boxes. This rotation is applied to the original axes, not to those currently displayed. When rotations are performed with the mouse, as mentioned in section 4.2 the boxes content is automatically updated. Rotations with respect of screen axes can be animated by checking the pertaining boxes. The *Start* (*Stop*) button toggles the animation. This feature can be combined with the *Record animation* option of section 4.7 to capture frames and making movies. In this case, animation ends when recording finishes.



Figure 79: Rotations menu

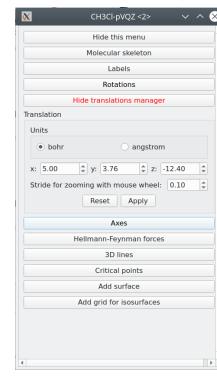


Figure 80: Translations menu

### 4.13.4 Translations

The *Translations* button opens a menu for translation manager –see fig 80. The components of the translation vector are displayed in three boxes which are synchronized with the translations carried out by mouse displacements, as commented in section 4.2. Changing the content of the boxes and pressing *Enter* on the keyboard or clicking *Apply* button carries out the translation specified in the boxes.

### 4.13.5 Axes

The *Axes* button opens a menu for molecular axes manager –see fig 81.

### 4.13.6 Hellmann-Feynman forces

The *Hellmann-Feynman forces* button opens a menu for displaying Hellmann-Feynman forces on nuclei –see fig 82. H-F forces are computed with the pertaining module of right menu –see 2.10– and stored in *.forces* files.



Figure 81: Molecular axes menu

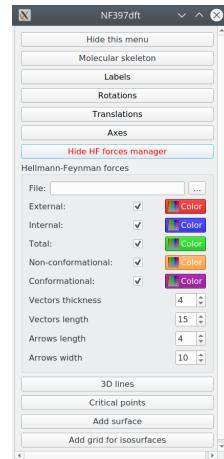


Figure 82: HF forces menu

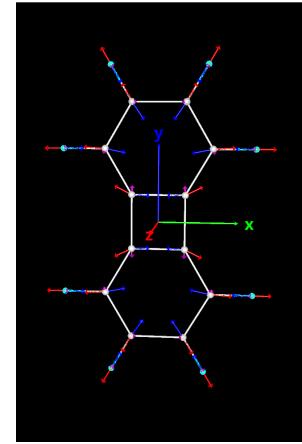


Figure 83: HF forces and molecular axes

#### 4.13.7 3D lines

The *3D lines* button displays a menu for loading and managing lines in space –see fig 84– which can be either electric field lines, density gradient, or MED or MESP gradient path lines computed with the suitable DAMQT programs as described in chapter 2 of this manual. Files extensions are *.cam* for electric field, *.dengr* for density gradient, *-d.gpdat* for MED gradient path, and *-v.gpdat* for MESP gradient path. Lines can be shown in the viewer –fig 85– by checking the appropriate box in the menu.



Figure 84: Field lines menu

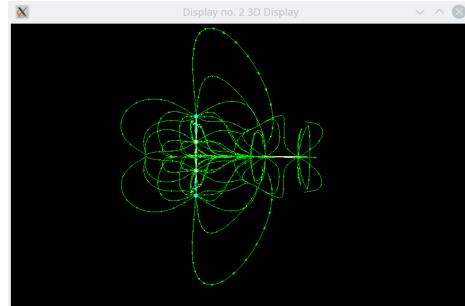


Figure 85: Field lines display

#### 4.13.8 Critical points

The *Critical points* button displays a menu for loading and managing MED or MESP critical points –see fig 86. File names are ended in *-cps-d.xyz* for MED CPs, and *-cps-v.xyz* for MESP CPs.



Figure 86: Critical points menu

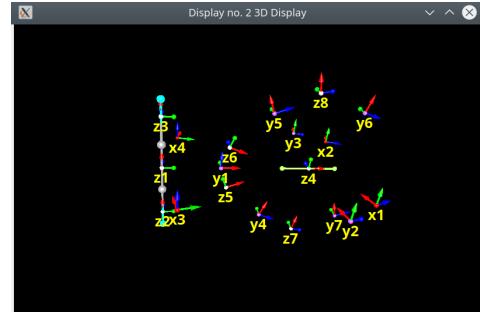


Figure 87: Hessian eigenvectors at critical points

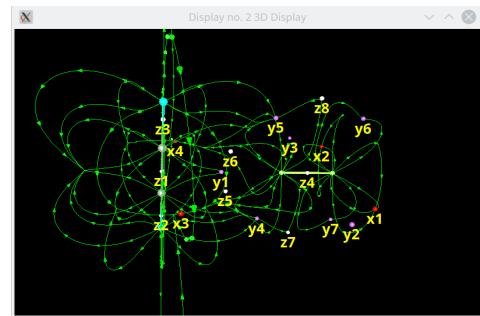


Figure 88: Critical points and field lines

Indices, symbols and field values of the CPs can be shown/hidden by checking/unchecking the corresponding boxes, and the number of figures in field value display can be changed in the *Precision* box. The following symbols convention hold: *x* refers to  $(+3, +3)$  CP, *y* to  $(+3, +1)$ , *z* to  $(+3, -1)$ , and *m* to  $(3, -3)$ .

To display selected CPs, check the box labeled *Only selected CPs* and choose the CPs to be displayed by double clicking on them. Double clicking on a CP toggles between hide/show. Fonts and colors can be changed clicking on the respective buttons. Numeration of CPs is independent of atoms numbering. A single set of indices is used for all CPs: *x*-type CPs are numbered first, followed by *y,z,m*-types.

*Hessian eigenvectors* menu controls display of eigenvectors of Hessian matrix on CPs (see fig 86). Arrow headed eigenvector means emerging gradient path while sphere headed eigenvector indicates that the gradient path is terminating into the CP. Color and shape of arrows can be changed in the pertaining boxes.

Critical points can be displayed together with surfaces or lines –see fig 88.

#### 4.13.9 Surfaces

The *Load surfaces* button displays a menu for loading surfaces generated with the programs described in section 2. In particular sigma hole surfaces, with extensions *.sgh* or *.srf*, MED or MESP basins borders,

with extension *.basins*, and high quality isodensity (*.isoden*) or isopotential (*.isopot*) surfaces can be visualized (see section 4.13.10 for high quality surfaces).

When a surface is loaded, an entry is added to the editor with three buttons which allow us to *Edit*, *Hide* or *Delete* it –see fig 89. If the *Edit* button is pressed, a menu is displayed whose content depends on whether basins borders –see fig 90– or sigma hole surfaces are loaded –see fig 91. The button label changes to *Close* and, if pressed again, all the surfaces menus are closed.

Pushing the *Hide* button, the surface is hidden, and the button label is changed to *Show*. Pressing it again causes the surface to be displayed.

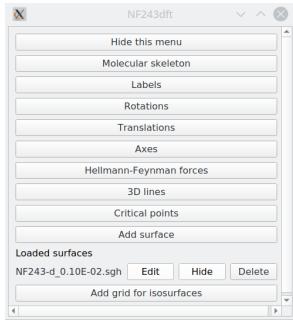


Figure 89: Surfaces menu

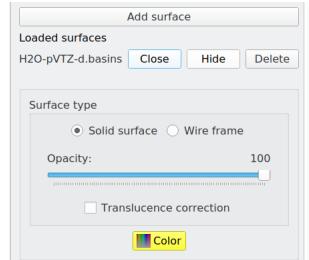


Figure 90: Basins options

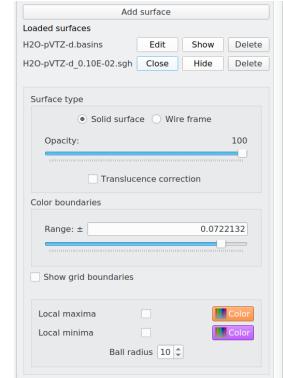


Figure 91: Sigma hole options

In case of sigma hole surfaces, local maxima and minima higher than a given threshold can be displayed, including optionally their symbols, indices, MESP values and coordinates, as shown in fig 93.

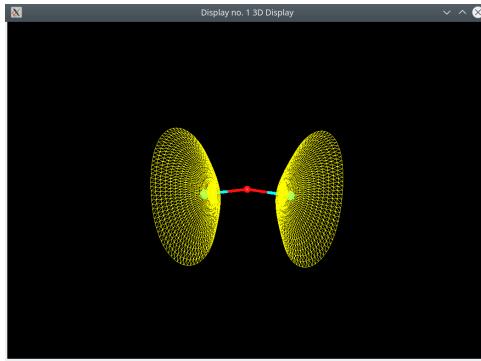


Figure 92: Basins borders

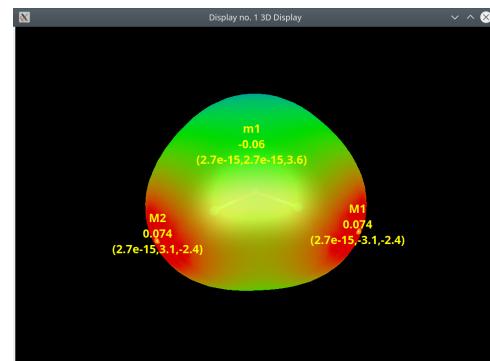


Figure 93: Sigma hole surface

Maxima are labeled with letter *M* (capital M) and minima with *m* (lowercase m), and MESP values and coordinates are quoted in atomic units. Several surfaces can be loaded together, and show/hide can be toggled by pressing the corresponding button.

#### 4.13.10 Isosurfaces

Another type of surfaces different than those treated in the previous section can be visualized, namely MED, MESP or molecular orbitals isosurfaces. To proceed, it is necessary first to load a grid where MED,

MESP or MOs are tabulated. These grids can be generated as mentioned in section 2. The *Add grid for isosurfaces* button must be pressed, opening a window for navigation to seek for a suitable grid file, with extension *.plt*.

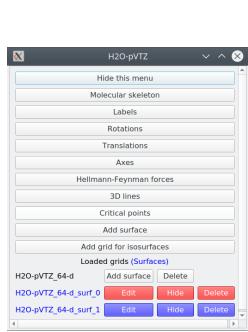


Figure 94: Grids for isosurfaces

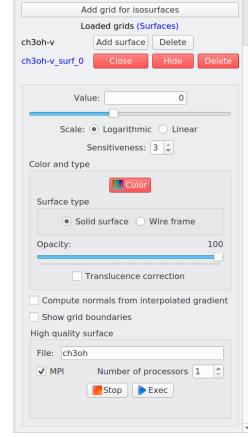


Figure 95: Isosurface menu

When the grid file is loaded, two buttons appear in the molecule menu, labeled as *Add surface* and *Delete*, which allow us to set a new isosurface or delete the grid and all its associated isosurfaces. Each time the *Add surface* is pressed, a new entry appears in the menu corresponding to the surface –see fig 94– with three new colored buttons: *Edit*, *Hide*, *Delete*. Pressing the first button, a menu for specifying the isovalue and handling the isosurface to be generated and displayed will appear –see fig 95.

The isovalue (in a.u.) must be supplied either by typing it in the top box or with the aid of the slider beneath. Both box values and slider are synchronized. The scale of the slider can be toggled between *logarithmic* and *linear*, and its sensitiveness adjusted to facilitate fine tuning. When typing the value in the box, the **Intro** key must be pressed in the keyboard to apply the change.

The surface color can be changed by pressing the corresponding button, which will open a palette window, and this change will be made also in the buttons associated to the surface in the molecule menu, thus facilitating the identification between buttons and surfaces when more than one isosurface is loaded. Furthermore, the grid boundaries can be visualized by checking the pertaining box.

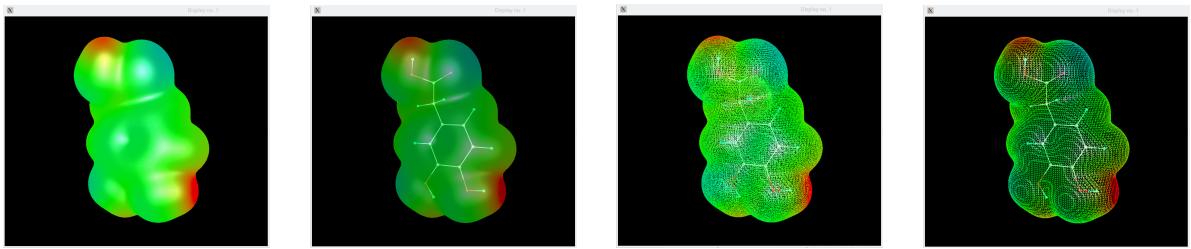


Figure 96: Surface display modes. From left to right: solid, solid with transparency, wired, wired with transparency and translucency correction.

Surfaces display can be toggled between *Solid* and *Wire frame* modes. The *Opacity* option controls the transparency degree of the surface and, in some cases, the effect can be improved by the checking the

*Translucence correction* box. This is particularly useful in *wire frame* mode, when dense meshes are displayed. In this case, combining the translucence correction with an opacity different from 1 improves the quality of the image, as shown in fig 96.

If grids with the pertaining gradient components are available (see sections 2.3 to 2.5), a check box will appear to enable gradient interpolation. In this case, the surface normals will be computed by interpolating the gradient values tabulated in the same grid points. This feature provides reasonably good normals in case that the variations of tabulated gradient components along the grid are smooth. Otherwise, strange patterns will be observed. In this case, it is possible to generate high quality surfaces, using the pertaining option at the bottom of the menu. When this option is selected, an analytical calculation of the normals in the vertices of the surface triangles is launched. The surfaces thus generated are stored in a file with extension *.isoden* for isodensity surfaces and *.isopot* for isopotential surfaces. These surface files can be loaded using the *Add surface* option of section 4.13.9.

Isosurfaces corresponding to different grids can be loaded together and isosurfaces can be combined with other surfaces, critical points and field lines.

## 4.14 Mouse operation

The 3D viewer supports the mouse events summarized below.

- Holding the *left button*, horizontal mouse displacements cause rotation around the space-fixed *y* axis (screen vertical), and vertical displacements, rotation around the space-fixed *x* axis (screen horizontal).
- Holding the *right button*, mouse displacements cause rotation around the space-fixed *z* axis (screen perpendicular).
- Holding together the **Shift** key and *left button*, horizontal mouse displacements cause translation along the space-fixed *x* axis, and vertical displacements, translation along the space-fixed *y* axis.
- Holding together the **Shift** key and the *right button*, mouse displacements cause translation along the space-fixed *z* axis (*zooming*).
- Holding the **Ctrl** key and double clicking on a molecule structure or surface toggles molecule activation. If more than one molecule is present in the region, it operates on the molecule loaded first.
- Double clicking the *left button* on a nucleus toggles atom selection. This action takes effect when the *Only selected* box is checked in the *Labels* menu of the molecule editor 4.13.2.
- Double clicking the *left button* on a critical point toggles its selection. This action takes effect when the *Only selected CPs* box is checked in the *Critical points* menu of the molecule editor 4.13.6.
- Double clicking the *left button* on a local extremum toggles its selection. This action takes effect when the *Only selected extrema* box is checked in the *Surfaces* menu of the molecule editor 4.13.7.
- Holding the **Shift** key and double clicking the *left* or *right button* opens a window to choose the index of an atom or critical point (when critical points are loaded) to toggle its selection –see figs 97 and 98. Accepting the action has the same effect as clicking directly on the nucleus or critical point.

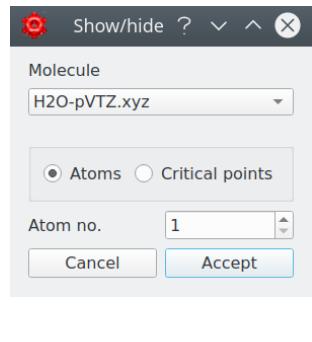


Figure 97: Atom selection

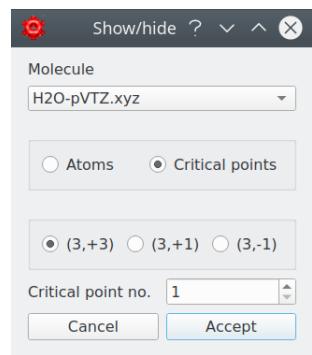


Figure 98: CP selection

In *Geometry measures* menu, when any of the options *Distances*, *Angles* or *Dihedral angles* is selected:

- Holding the **Shift** key while double clicking the *left button* on a nucleus or critical point selects it for suitable measurement. Measurement is only allowed between centers belonging to the same molecule.
- In case of *Distances*, when distances labels are shown in the viewer, clicking on a label removes the corresponding distance measurement.

## 5 Interfaces

The current version of DAMQT includes built-in interfaces for automatic generation of *.den* and *.ggb*s files from files created by GAUSSIAN, MOLPRO, TURBOMOLE, MOPAC, and NWChem packages, as well as those with MOLEKEL format. In all cases, the interface is invoked by just clicking on a suitable file generated by one of these programs. Here follows the requirements and usage of each interface.

### 5.1 GAUSSIAN interface

The interface to GAUSSIAN uses the *.fchk* file that can be generated from the *.chk* file with GAUSSIAN's *formchk* utility. Since DAMQT only works with spherical functions, GAUSSIAN must be run with the *5D 7F* option. When attempting to use files coming from calculations which did not include that option, the interface will complain and stop.

To use the interface, press *Import data* button  and double click on a *.fchk* file. Then, press the  key.

### 5.2 MOLPRO interfaces

There are two different interfaces to MOLPRO included in the package. `MOLPRO_xml_interface.py` extracts information from MOLPRO's *.xml* files, whereas `MOLPRO_out_interface.exe` gets it from the standard output file (usu., *.out*).

To use `MOLPRO_xml_interface.py`, the *.xml* must be created with a suitable content and format. This can be done by including in MOLPRO's input file a line like:

```
{put,xml,fname_esf.xml;keepspherical}
```

where `fname_esf` stays for a suitable name. In this way, MOLPRO will generate two *.xml*, but the interface only works with the `fname_esf.xml`. When attempting to use an *.xml* without the appropriate format and content the interface will complain and stop.

The interface `MOLPRO_out_interface.exe` uses the standard output file generated in a calculation with MOLPRO. The output file must contain information on the geometry, basis set and density matrix. Therefore, the following options must be included in the input file to generate a suitable output:

```
gprint,basis
{matrop
load,d,den
print,d
}
```

If molecular orbitals are to be displayed, they must be written in MOLPRO's output file. The following code in the input file does the job:

```
gprint,basis
{matrop
load,orb
print,orb
}
```

In UHF calculations, the following codes allow us to write alpha orbitals:

```
{uhf;orbital,2100.2}
{matrop
load,orba,orb,2100.2,set=1
print,orba
}
```

or beta orbitals:

```
{uhf;orbital,2100.2}
{matrop
load,orbb,orb,2100.2,set=2
print,orbb
}
```

To use any of the interfaces, press *Import data* button  and double click on a *.out* or a suitably generated *.xml* file. Then, press the  key. When attempting to use files which have been not generated by MOLPRO or do not have the appropriate format, the interface will complain and stop. Usually, MOLPRO's standard output files provide molecular orbital coefficients and density matrix elements with a reduced number of figures. Furthermore, in cases of very high quality basis sets, more than six contractions may share the same primitives; this implies a format change in output file which causes **MOLPRO\_out\_interface.exe** to fail. To overcome these problems, two unofficial patches are supplied in the **utils** directory of the package: **arinp.F.diff** and **matrop.F.diff**. Running these patches, some output formats are changed in **arinp.F** (argos directory) and **matrop.F** (scf directory) increasing the number of figures in molecular coefficients and density elements, and preventing the above mentioned issue when very high quality basis sets are used.

Finally, it must be recalled that molecular orbitals attained in a UHF calculation are different in *.out* file from those of *.xml* file. In *.out* file they appear separated in two sets corresponding to positive and negative spin components, whereas in the *.xml* file natural orbitals are stored. As a consequence, the two interfaces will yield different orbitals.

**IMPORTANT:** in some cases, when dealing with systems with symmetry, MOLPRO yields wrong signs in some symmetry orbitals, leading to incorrect results. This can be noticed as an erroneous total electron charge when carrying out the DAM partition of density. This is a flaw in MOLPRO output file in these cases. The bug is fixed by running the **arinp.F.diff** patch.

### 5.3 ADF interface

The interface to ADF requires a calculation in which TAPE15 and TAPE21 need to be saved.

```
"$ADFBIN/adf" << eor
...
SAVE TAPE21 TAPE15
eor
```

The executable *adf2damqt*, included in ADF suite can be run with up to three optional arguments:

```
"\$ADFBIN/adf2damqt" {fname} {SPIN} {NOORBITALS}}
```

If a specific name (*fname*) is desired for the files generated by the interface, it must be supplied as first optional argument, and must not coincide with any of the two additional optional keywords: *SPIN* and *NOORBITALS*. Otherwise "ADF" is chosen as default root name (*fname*) for files generated by the interface, and files containing electron density matrix (*fname.den*) and molecular orbitals (*fname.SLorba* and, eventually, *fname.SLorbb*). These files will be created in a format suitable to be read by DAMQT. Two further optional keywords can be supplied:

*SPIN*: for storing spin density matrix in *fname.den* file (instead of total electron density, which is the default).

*NOORBITALS*: to prevent generation of files with molecular orbitals (by default orbitals are generated). *SPIN* and *NOORBITALS* are case insensitive and can be given in any order (but always after optional *fname* when required).

## 5.4 TURBOMOLE interface

The interface to TURBOMOLE uses the *.basis* , *.mos* , *.coords* and, optionally, *.control* files that are generated in a TURBOMOLE calculation. *.control* file is only necessary if charged systems are computed or UHF calculations are made. All these files must have a common name with the pertaining extensions to be accessed by the interface. This name will be used as default project name.

To use the interface, press *Import data* button  and double click on a *.basis* , *.mos* or *.coords* file. Then, press the  key.

If any of the mandatory files is absent, the interface will complain and stop.

## 5.5 MOPAC interface

The interface to MOPAC uses *.aux* files generated by MOPAC with the *AUX* keyword.

It must be recalled that MOPAC works only with valence electrons and the Zero Differential Overlap (ZDO) approximation. This implies that the total electron charge cannot be retrieved from a MOPAC calculation, and to retrieve the valence electron charge, only one-center densities must be taken into account in the MED partition, for consistency with the ZDO approximation.

To use the interface, press *Import data* button  and double click on a *.aux* file. Then, press the  key.

## 5.6 NWChem interface

The interface to NWChem extracts data from NWChem output files. To make the interface accessible by just clicking on the outputfile, it is necessary to set the output file extension as *.nwcout* . File with molecular orbitals (*\*.movec*) must be accesible and must have the same name as the (*\*.nwcout*) file.

**Important!!!** For the interface to work, the *mov2asc* executable must be available in directory *\$NWChem\_TOP/contrib/*, where *\$NWChem\_TOP* stands for the NWChem home directory. If the executable is in a different location create a symbolic link to it in the directory *\$NWChem\_TOP/contrib/*.

To use the interface, press *Import data* button  and double click on a *.nwcout* file. Then, press the  key.

## 5.7 MOLEKEL interface

The interface to MOLEKEL extracts data from MOLEKEL *.mkl* files.

To use the interface, press *Import data* button  and double click on a *.mkl* file. Then, press the  key.

## 6 Gallery

This section should be considered as a mere sketch of the possibilities that DAMQT offers in the analysis of the density and related properties, that hopefully may suggest further applications to user's imagination. The following pictures are intended as highlights to illustrate these possibilities and a way to interpret the results that DAMQT provides. Some conventions are followed in these drawings: electron density is plotted (not charge density, beware of sign); in density deformation plots: red color is used for positive deformations (charge accumulations with respect to the density resulting from the atomic spherical terms), blue color is used for negative deformations (charge depletion); in electrostatic potential: red color is used for positive values and blue color for negative values. Contour values given are ordered from innermost to outermost surfaces. Unless otherwise indicated, pictures correspond to densities computed at RHF level using Dunning's cc-QVTZ and cc-pVTZ basis sets<sup>9</sup>. All the plots correspond to grids computed at the medium resolution level (129x129x129) and have been captured in *jpg* format with the viewer *Capture* facility.

### 6.1 Molecular density

The most immediate application of DAMQT is the tabulation of the electron density in molecules. Using DAM partition, for large systems this tabulation may be faster than evaluation from density matrix and basis functions. Fig 99 shows the total density of CH<sub>3</sub>Cl (left plate) and the density corresponding to only spherical atomic terms (right plate).



Figure 99: Electron density of CH<sub>3</sub>Cl. *Left*: full density, *right*: only atomic spherical terms. Contour values: 20, 1, 0.2, 0.04

Furthermore, DAM partition allows to separate the atomic spherical terms from those corresponding to deformations. Fig 100 shows some density deformation contours for CH<sub>3</sub>Cl.



Figure 100: Density deformations of CH<sub>3</sub>Cl. *Left*: positive deformations (charge accumulation), *right*: negative deformations (charge depletion). Contour values:  $\pm 0.08, \pm 0.04, \pm 0.02, \pm 0.01$

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<sup>9</sup>cita a Dunning

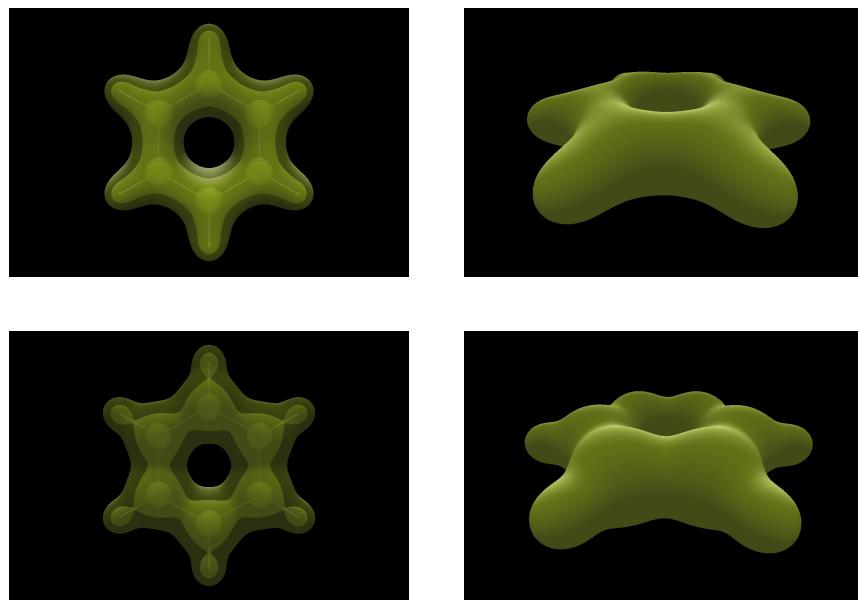


Figure 101: Electron density of  $C_6H_6$ . *Upper*: full density. *Lower*: only atomic spherical terms. Contour values: 0.8, 0.3, 0.2, 0.1 (only 0.1 in right plates).

Figures 101 and 102 show some contour density and density deformations surfaces for benzene.

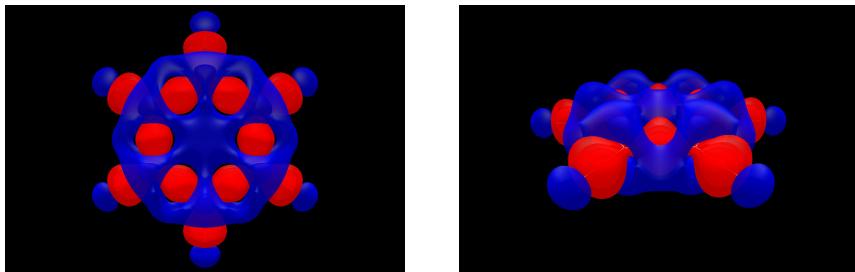


Figure 102: Density deformations of  $C_6H_6$ . *Red*: positive deformations (charge accumulation), *blue*: negative deformations (charge depletion). Contour values: 0.09, 0.05,  $\pm 0.03$ ,  $\pm 0.01$

## 6.2 Atoms in molecules

Another application of DAMQT is the analysis of the atomic components of the density as defined in DAM partition. Figures 103 and 104 show the full atomic density and its related deformations for chlorine and carbon atoms in  $CH_3Cl$ .

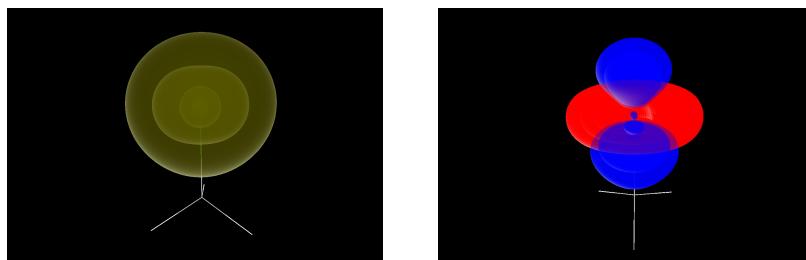


Figure 103: Atomic density of Cl in  $\text{CH}_3\text{Cl}$ . *Left:* electron density, contour values: 20, 1, 0.2, 0.04; *right:* deformation, contour values: 0.1, 0.02,  $\pm 0.01$ ,  $\pm 0.005$



Figure 104: Atomic density of C in  $\text{CH}_3\text{Cl}$ . *Left:* electron density, contour values: 5, 1, 0.2, 0.04; *right:* deformation, contour values: 0.05, 0.02,  $\pm 0.01$ ,  $\pm 0.005$

### 6.3 Density deformation and bonding

Deformation patterns of atoms in different molecular environments can be also used to characterize different types of bonds.

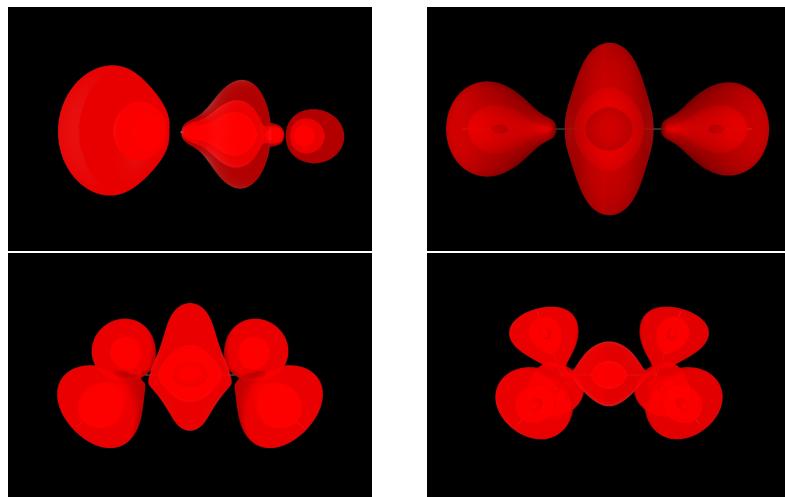


Figure 105: Positive density deformations (charge accumulation) *Upper left:*  $\text{CO}$ , *upper right:*  $\text{C}_2\text{H}_2$ , *lower left:*  $\text{C}_2\text{H}_4$ , *lower right:*  $\text{C}_2\text{H}_6$ . Contour values: 0.09, 0.05, 0.01.

Figure 105 shows the charge accumulation (positive deformation) in four molecules containing carbon

with different bond types. Figure 106 shows the deformation pattern in CO and C<sub>2</sub>H<sub>2</sub> including contours of charge depletion (negative deformation).

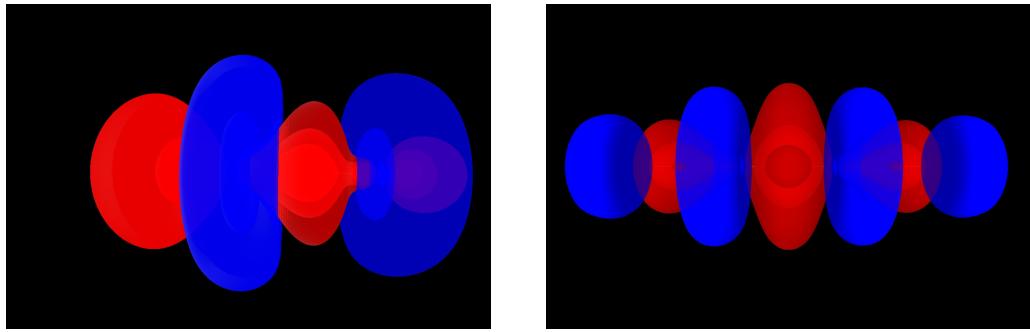


Figure 106: Density deformations (charge accumulation) in CO (*left*) and acetylene (*right*). Contour values: 0.09, 0.05,  $\pm 0.01$ .

In conjugated systems, it is also interesting to look at the deformations corresponding to contour values lower than those considered so far. Figure 107 shows the positive density deformation (charge accumulation) in C<sub>6</sub>H<sub>6</sub> at low contour values. These plots correspond to high resolution grids (257x257x257) of a RHF density computed with Dunning's cc-pVQZ basis set.

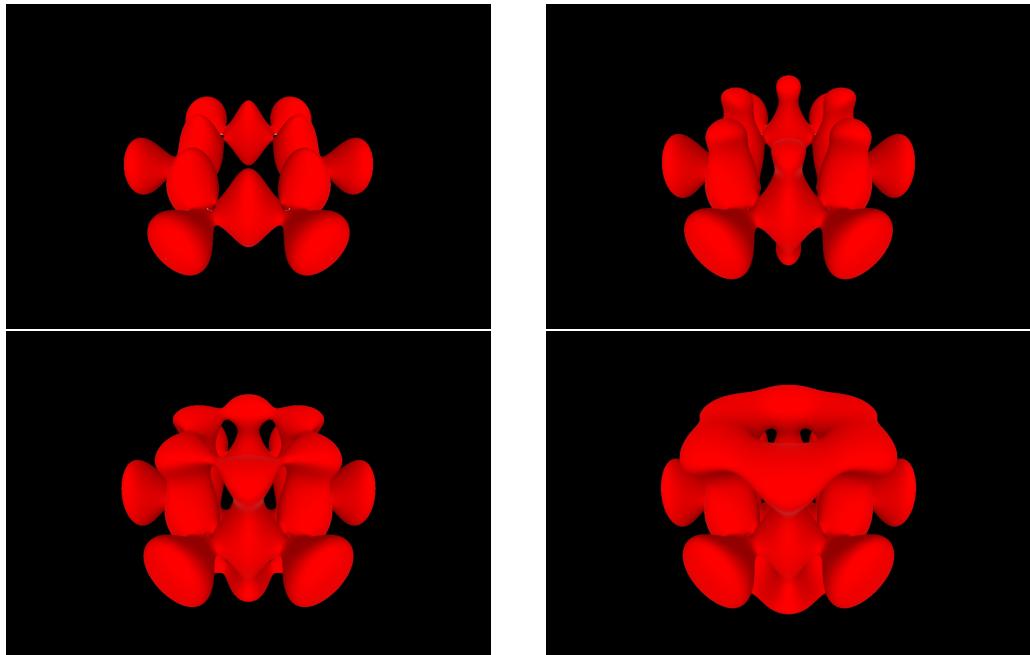


Figure 107: Positive density deformations (charge accumulation) in C<sub>6</sub>H<sub>6</sub>. Contour values: 0.005, 0.002, 0.0015, 0.001.

## 6.4 Electrostatic potential

DAMQT also enables a fast evaluation of electrostatic potential, without appealing to the representation of the density in terms of point multipoles (*long-range expansion*). Figure 108 shows some electrostatic

potential contours of  $\text{H}_2\text{O}$  and  $\text{NH}_3$  in the regions of negative (blue) and positive (red) potential values drawn from a high resolution grid (257x257x257). Positive and negative regions are separately plotted for  $\text{CH}_3\text{Cl}$  in figure 109.

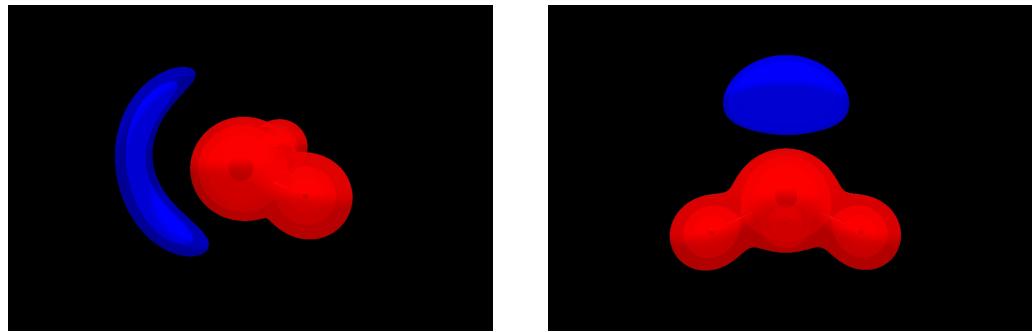


Figure 108: Electrostatic potential of  $\text{H}_2\text{O}$  (*left*) and  $\text{NH}_3$  (*right*). Contours: *red*: 15, 2, 1, 0.5, *blue*: -0.085, -0.080.



Figure 109: Electrostatic potential of  $\text{CH}_3\text{Cl}$ . *Left*: positive region, contours: 5, 0.5, 0.05, 0.01. *Right*: negative region, contours: -0.025, -0.020, -0.015

## 6.5 Molecular topography

A fast and efficient topographical analysis of both electron density and electrostatic potential can be performed in DAMQT. Topography involves mapping of critical points, determination of molecular graph (constituted by atomic interaction lines) and atomic basins. The molecular graph and atomic basin in the field of MESP are termed as MESP-based Topograph and MESP-based atomic basins respectively. Figure 110 shows MESP critical points of  $\text{H}_2\text{O}$  and  $\text{NH}_3$  where the red, green and grey dots denote  $(3, +3)$  CP,  $(3, +1)$  CP and  $(3, -1)$  CP respectively. The eigenvectors of each of the critical points are also displayed in different colors as well as type. Color of eigenvector is determined by the absolute value of the magnitude of eigenvalue to which it is associated. *i.e.* Eigenvector associated to largest eigenvalue (*abs.* magnitude) is represented by red color. This is followed by blue and green colored eigenvectors reflecting the decreasing magnitude of associated eigenvalue. The positivity or negativity of

the eigenvalues are accounted by an arrow-headed or a sphere-headed eigenvector respectively.

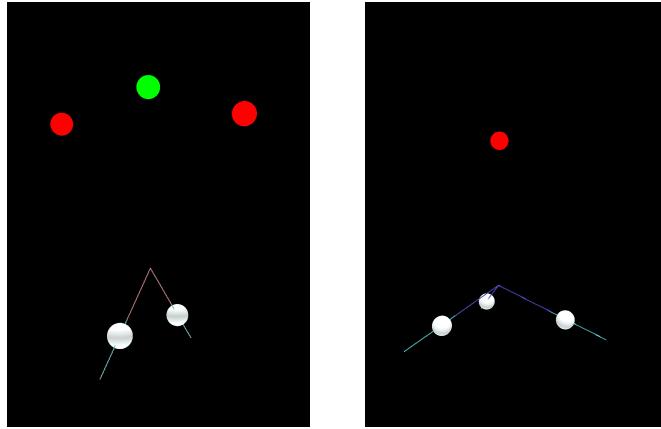


Figure 110: MESP critical points of H<sub>2</sub>O (*left*) and NH<sub>3</sub> (*right*). (3,+3) CP: *red*; (3,+1) CP: *green*; (3,-1) CP: *grey*.

Figure 111 shows MESP-based topographs of H<sub>2</sub>O and NH<sub>3</sub>. These gradient field lines connecting various critical points and nuclei are constructed in the directions of maximum change of potential.

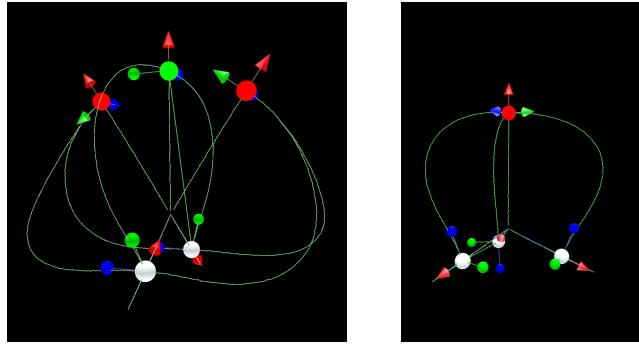


Figure 111: MESP-based topographs of H<sub>2</sub>O (*left*) and NH<sub>3</sub> (*right*). Eigenvectors show the direction of maximum change of function value at the critical points.

Figure 112 shows MESP atomic basins of H<sub>2</sub>O and NH<sub>3</sub>. The oxygen atom in H<sub>2</sub>O and nitrogen atom in NH<sub>3</sub> possess closed zero flux surfaces, whereas the hydrogens show open surfaces.

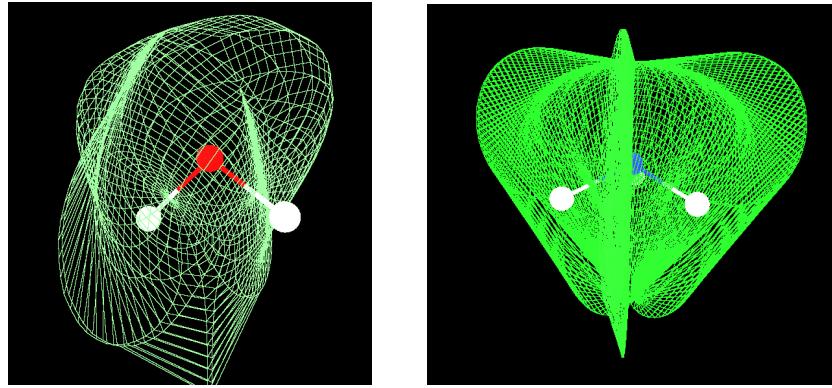


Figure 112: MESP-based atomic basins of  $\text{H}_2\text{O}$  (*left*) and  $\text{NH}_3$  (*right*).

## 6.6 MESP sigma hole

MESP sigma hole can be computed over a MED isosurface of user-defined density value. Figure 113 shows the MESP sigma hole of benzoic acid over the MED isosurface of density  $0.001 \text{ bohr}^{-3}$ . The MESP maximum (over the acid proton) and the minimum are displayed together with their MESP values.

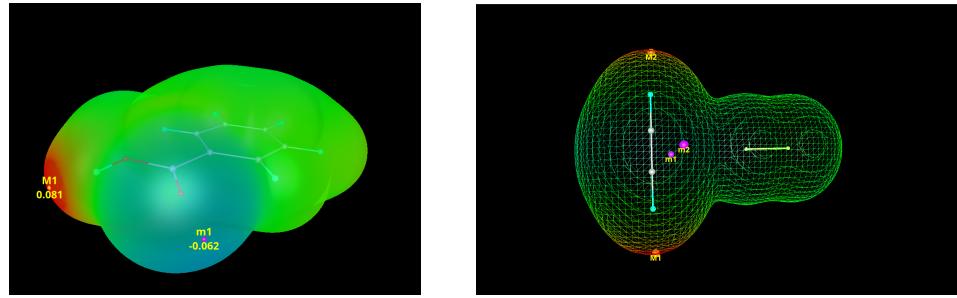


Figure 113: MESP extrema on sigma hole of Benzoic acid (*left*) and system HCCH-F<sub>2</sub> (*right*)

## 6.7 Electric field

Electric field can be also efficiently computed with DAMQT, and 3D plots of the corresponding lines can be drawn at low cost. Figure 114 shows two different views of the field lines of  $\text{H}_2\text{O}$ .

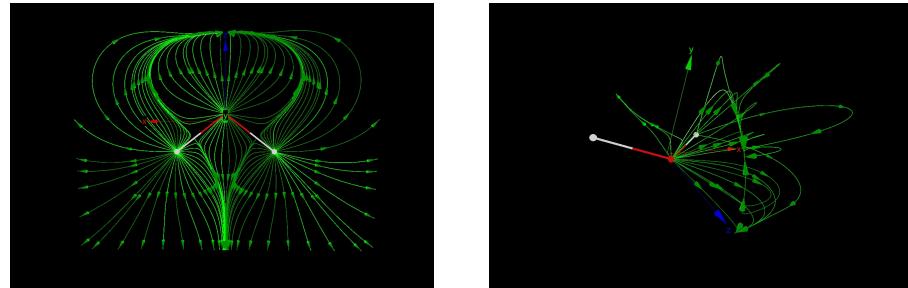


Figure 114: Electric field lines in  $\text{H}_2\text{O}$

Relationship between the different types of MESCP critical points and electric field lines is clearly shown in fig 115.

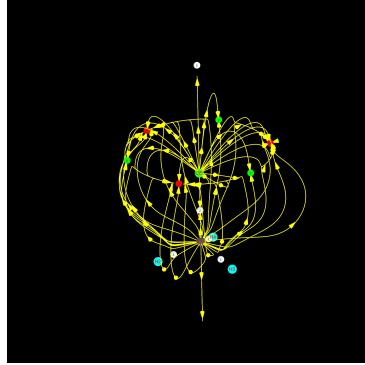


Figure 115: MESCP critical points of  $\text{CH}_3\text{Cl}$  and electric field lines starting from carbon and chlorine.

## 6.8 Hellmann-Feynman forces

DAMQT also gives a decomposition of the Hellmann-Feynman forces acting on the nuclei in terms of internal (*self-pulling*) and external components. The internal force on a nucleus is the force caused by its own atomic electron density. The external force is caused by the electron clouds of the remaining atoms and the charges of the other nuclei.

Figure 116 shows the decomposition of the Hellmann-Feynman forces provided by DAMQT in 4-amine pyridine. Left plate shows a significant total component of the force on the N atom of the pyridine ring. Right plate shows a conformational force on this atom which almost coincides with the total force. The origin of such force can be attributed either to a lack of geometry optimization or to an insufficient fulfillment of the Hellmann-Feynman theorem by the cc-pVTZ basis set.

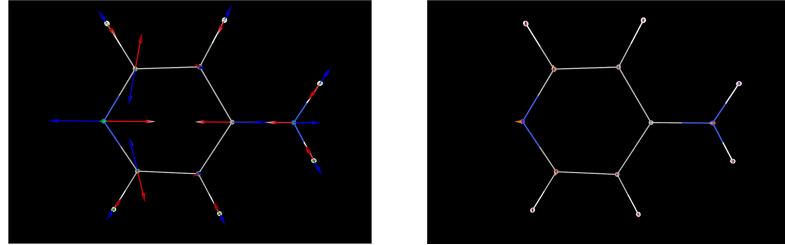


Figure 116: Hellmann-Feynman forces in 4-amine pyridine. *Left:* Internal (red), external (blue) and total (green) forces. *Right:* conformational (orange) and non-conformational (purple) forces.

## 6.9 Zernike-Canterakis expansion of MED

One-center expansions of MED have been proposed as a source of MED fingerprints for molecular pattern recognition. DAMQT can be used to carry out expansions in terms of Zernike-Canterakis functions as well as Jacobi functions of MED. Upper left panel of figure 117 shows a 2D plot of biphenyl MED which can be compared with the Zernike-Canterakis expansions for different levels of expansion, as shown in the remaining panels. As it can be appreciated, one-center expansions give curly surfaces in the region of low values of MED, in an attempt to reproduce nearly zero values in terms of polynomials.

3D views of the density are collected in figure 118 for contour values of density equal to  $0.1 \text{ bohr}^{-3}$  and  $0.03 \text{ bohr}^{-3}$ . Left plates correspond to exact density (with DAM expansion) and right plates to Zernike-

Canterakis expansion. Surfaces corresponding to a contour value of  $-0.03 \text{ bohr}^{-3}$  in Zernike-Canterakis expansions are depicted in blue. Notice that negative values should not appear since density is a positive definite function. These values are artifacts coming from the truncation in expansion and give an idea of the accuracy. The changes of sign in these expansions for the lower contour are the 3D counterparts of the oscillations mentioned in 2D plots.

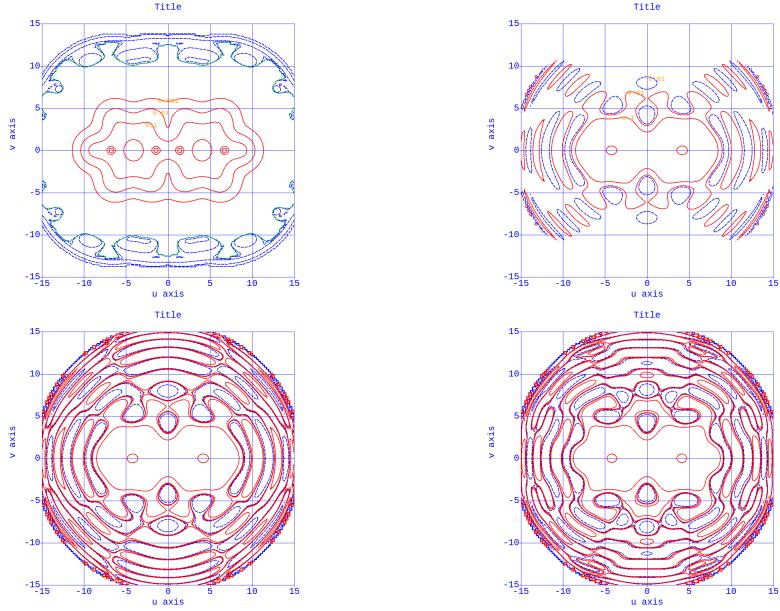


Figure 117: MED of biphenyl: upper-left: DAM expansion, remaining panels: Zernike-Canterakis expansions with different lengths

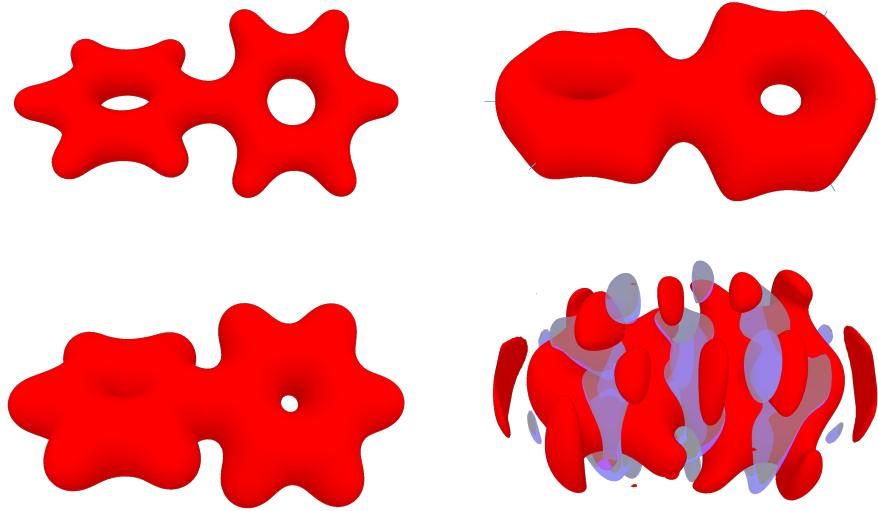


Figure 118: MED of biphenyl: left: DAM expansion, right: Zernike-Canterakis expansions; upper: contour  $0.1 \text{ bohr}^{-3}$ , lower: contour  $0.03 \text{ bohr}^{-3}$  (in blue: contour  $-0.03 \text{ bohr}^{-3}$ )

## A Appendix: Format of files *.ggbs* and *.den*

The *.ggbs* file is a text file containing the input corresponding to the geometry and GTO basis set. It must be written in free format style and organized as follows (see fig 119):

Figure 119: *.ggbs* file structure

NCEN	Number of centers
X1 Y1 Z1 ZNUC1 X2 Y2 Z2 ZNUC2 ...	Cartesian coordinates in bohr and nuclear charge of centers
NCONTR1	Number of contractions on first center
NPRIM11 L11 EXP111 EXP112 EXP113 ... COEF111 COEF112 COEF113 ... ...	First contraction
NPRIM12 L12 EXP121 EXP122 ... COEF121 COEF122 ... ...	Second contraction
NCONTR2	Number of contractions on second center
NPRIM21 L21 EXP211 EXP212 EXP213 ... COEF211 COEF212 COEF213 ... ...	First contraction
NPRIM22 L22 EXP221 EXP222 ... COEF221 COEF222 ... ...	Second contraction

First record: number of centers (*ncen*, integer)

Second and following *ncen* records: Cartesian coordinates in bohr and nuclear charge of each center ( $x_i, y_i, z_i, znuc_i$ ; 4 (real\*8) )

The following records will contain the basis set for each center *i* organized as:

One record with the number of contracted functions (*ncontr<sub>i</sub>*, integer) associated to the center followed, for each contracted function, by:

- one record with the number of primitives (*nprim<sub>i,j</sub>*, integer) and the *l* quantum number associated to the contraction (*l<sub>i,j</sub>*, integer)
- as many records as required with the primitive exponents (*exp<sub>i,j,k</sub>*, real\*8)
- as many records as required with the contraction coefficients (*coef<sub>i,j,k</sub>*, real\*8)

The *.den* file is also a text file containing, in free format, one leading record with the number of basis functions (integer) followed by as many records as required to load the elements of the lower triangle of the full density matrix sequentially stored (real\*8).

## B Appendix: Files *\_2016.damqt*

Files *\_2016.damqt* are unformatted files which contain the data for the piecewise representation of the radial factors. Since this information may be useful for other applications different than those developed in DAMQT, a brief description of the structure of this file is given.

Furthermore, the radial factors  $\rho_{lm}^A(r)$  are piecewise fitted to products of exponentials times Chebyshev polynomials,  $T_k(t)$ :

$$\rho_{lm}^A(r) \simeq e^{-\xi_i r} \sum_{k=0}^{n_i} c_k^{(i)}(l, m) T_k(t) \quad (1)$$

in a set of intervals defined by  $\lambda_{i-1} \leq r \leq \lambda_i$ ;  $i = 1, \dots, n$ , and the variable  $t$ , by:

$$t \equiv 2 \frac{r - \lambda_{i-1}}{\lambda_i - \lambda_{i-1}} - 1 \quad (2)$$

up to  $\lambda_{max} = 20$  bohr.

Notice that coefficients are sequentially stored for only nonvanishing radial factors. A pointer, ICFPOS, is used to locate the expansion coefficients of the radial factor corresponding to a pair of quantum numbers  $(l, m)$  in a given center. Negligible radial factors repeat the ICFPOS value of the previous non-vanishing factor. Thus, since loops in programs run from the index pointed by an element of ICFPOS to that pointed by the next element minus one, in vanishing radial factors these loops are skipped (because second index is lower than first one).

Data are stored by centers, and the storage order is as follows. For each center, ICFPOS array is stored first, followed by fitting exponents ( $\xi_i$ ), and next, by expansion coefficients ( $c_k^{(i)}(l, m)$ ).

An ancillary program: `readdamqt320.F90` which enables to read the content of the *\_2016.damqt* files to plain text files is included in the package. To run it, just type `readdamqt320.exe` and you will be prompted to supply the name of the *\_2016.damqt* file to be read.

## C Appendix: Files *.plt* and *.pltd*

Files *.plt* and *.pltd* are binary files which contain data tabulated on a 3D grid. They are intended for 3D plotting of density, density deformations, electrostatic potential and molecular orbitals. Files *.pltd* contain their derivatives.

An ancillary program: `readplt320.F90` which enables to read the content of the *.plt* or *.pltd* files to plain text files is included in the package. To run it, just type `readplt320.exe` and you will be prompted for the name of the *.plt* or *.pltd* file to be read.

A program `subtractplt320.F90` is also supplied to subtract the values corresponding to two different *.plt* files. Both *.plt* files must correspond to the same grid, otherwise the program will complain and stop. To run the program, type `subtractplt320.exe` and you will be prompted for the names of the *.plt* files. Values of the second file will be subtracted from those in the first one.

## D Appendix: Files *.cnt*

Files *.cnt* are binary files which contain data tabulated on a 2D grid. They are intended for 2D plotting of density, density deformations, electrostatic potential and molecular orbitals, as well as their derivatives. An ancillary program: `readcnt.F90` which enables to read the content of the *.cnt* files to plain text files is included in the package. This program also generates a file with a format suitable to be plotted with `gnuplot`. To run it, just type `readcnt.exe` and you will be prompted for the name of the *.cnt* file to be read.

## E Appendix: Files SGMESP\_summary.txt

Files `SGMESP_summary.txt` are text files which contain a summary of statistic parameters of MESP on a density isosurface. The following parameters are included in strict order:

**Total area,  $\mathcal{A}$ :** area of density isosurface in bohr<sup>2</sup>.

**Volume,  $\mathcal{V}$ :** volume enclosed by the density isosurface in bohr<sup>3</sup>.

**MESP max,  $V_M$ :** highest value of MESP on the density isosurface.

**MESP min,  $V_m$ :** lowest value of MESP on the density isosurface.

**kntmax:** number of disjoint regions with maxima.

**kntmin:** number of disjoint regions with minima.

**xmin:** lowest value of  $x$  coordinate of density isosurface vertices.

**xmax:** highest value of  $x$  coordinate of density isosurface vertices.

**ymin:** lowest value of  $y$  coordinate of density isosurface vertices.

**ymax:** highest value of  $y$  coordinate of density isosurface vertices.

**zmin:** lowest value of  $z$  coordinate of density isosurface vertices.

**zmax:** highest value of  $z$  coordinate of density isosurface vertices.

**Positive area,  $\mathcal{A}^+$ :** area of density isosurface with positive MESP values, in bohr<sup>2</sup>.

**Negative area,  $\mathcal{A}^-$ :** area of density isosurface with negative MESP values, in bohr<sup>2</sup>.

**MESP mean,  $\bar{V}$ :** average value of MESP on isosurface ( $\Omega$ ) in au (Hartree/e).

**Positive MESP mean,  $\bar{V}^+$ :** average value of MESP on density isosurface with positive MESP ( $\Omega^+$ ) in au (Hartree/e):

**Negative MESP mean,  $\bar{V}^-$ :** average value of MESP on density isosurface with negative MESP ( $\Omega^-$ ) in au (Hartree/e).

**MESP variance,  $\sigma^2$ :** variance of MESP on isosurface in au<sup>2</sup> (Hartree<sup>2</sup>/e<sup>2</sup>).

**Positive MESP variance,  $(\sigma^+)^2$ :** variance of MESP on isosurface with positive MESP values in au<sup>2</sup> (Hartree<sup>2</sup>/e<sup>2</sup>).

**Negative MESP variance,  $(\sigma^-)^2$ :** variance of MESP on isosurface with negative MESP values in au<sup>2</sup> (Hartree<sup>2</sup>/e<sup>2</sup>).

**MESP deviation,  $\Pi$ :** mean of MESP deviations (sum of absolute differences between point and mean values) in au (Hartree/e).

**$\nu$  parameter:**  $\nu = (\sigma^+)^2 / (\sigma^-)^2 / (\sigma^2)^2$ .

Average values, variances and deviation are computed by integration of the pertaining properties in the triangles defining the isosurface. MESP is linearly fitted in each triangle using the values in the vertices, and the integrals are carried out analytically using the fitted functions.

In the following expressions,  $\Omega$ ,  $\Omega^+$ ,  $\Omega^-$  denote the corresponding total or partial isosurfaces.

$$\bar{V} = \frac{1}{\mathcal{A}} \int_{\Omega} V(\mathbf{r}) dS \quad \bar{V}^+ = \frac{1}{\mathcal{A}^+} \int_{\Omega^+} V(\mathbf{r}) dS \quad \bar{V}^- = \frac{1}{\mathcal{A}^-} \int_{\Omega^-} V(\mathbf{r}) dS$$

$$(\sigma^+)^2 = \frac{1}{\mathcal{A}^+} \int_{\Omega^+} [V(\mathbf{r}) - \bar{V}^+]^2 dS \quad (\sigma^-)^2 = \frac{1}{\mathcal{A}^-} \int_{\Omega^-} [V(\mathbf{r}) - \bar{V}^-]^2 dS \quad \sigma^2 = (\sigma^+)^2 + (\sigma^-)^2$$

$$\Pi = \frac{1}{\mathcal{A}} \int_{\Omega} |V(\mathbf{r}) - \bar{V}| dS$$

## F Appendix: Hints for cluster building with EPIC

Building a cluster with EPIC can be a convoluted task unless some systematic procedure is followed. Here we propose some steps that may be helpful for this purpose, starting from scratch.

The preliminary steps are common to other DAMQT applications, and they will be just mentioned without much detail. We will focus here in what are more specific tasks for cluster optimization using EPIC.

1. Select which molecule will play as *host* and which other will be treated as guests in the cluster (both could be the same). This distinction is important, as more information is required for host than for guests.
2. Start a project from a molecular calculation for the host with any standard package compatible with DAMQT.
3. Carry out the DAM analysis –sec 2.2– and compute the MESP critical points –sec 2.6.
4. Open a 3D viewer and load the host molecule in the canvas.
5. To **generate the cluster from canvas**, guest molecules must be loaded by means of their *.xyz* geometry files, and displaced to suitable starting positions. Displaying some geometric parameters (distances or angles) may be helpful in this regard –see fig 120.

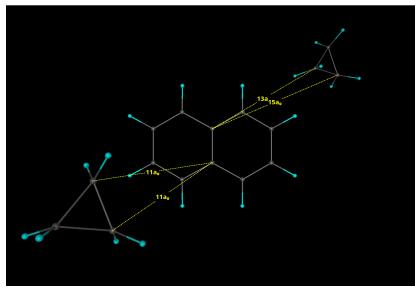


Figure 120: Loading molecules for cluster

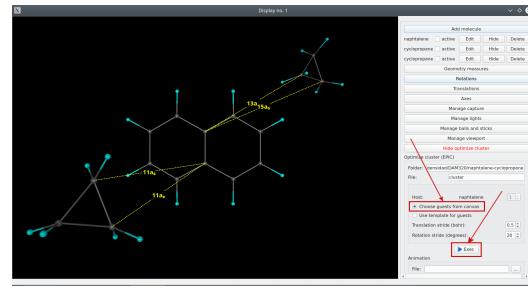


Figure 121: Cluster optimization from canvas

6. Remember that translations and rotations act on the active molecules. Activation can be toggled in the corresponding checkbox or with mouse, by **Ctrl + Double click**. When more than one molecule (either active or inactive) are placed in the same region, the latter action only operates on the molecule loaded first.
7. Deactivating all molecules, the system can be translated or rotated as a whole. You can use this fact for improving perception of the actual positions.

8. With the option *Choose guest from canvas* checked, press the *Exec* button –see fig 121– to start optimization.
9. Previously loaded molecules will be hidden, the cluster will be loaded in the canvas, and its evolution will be displayed from the starting geometry through the intermediate ones while optimization is in progress. This will be accompanied by a message on the bottom left of the window during the optimization –see fig 122.
10. A box with a message will be displayed when optimization finishes –see fig 123. It is important to wait until this message appears, to ensure that the process has been completed.

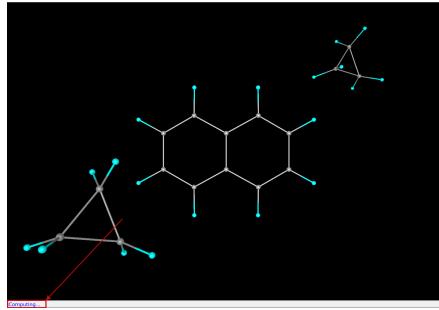


Figure 122: Optimization in progress

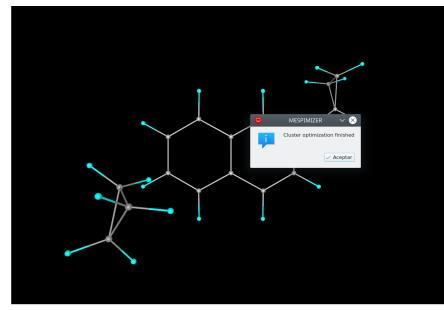


Figure 123: End of optimization

11. A file *\*.xyz\_frames* has been created, containing the geometries at the starting, intermediate and ending positions. The path and name of this file are supplied in suitable boxes –see fig 124.
12. File *\*.xyz\_frames* can be used for animation by loading it in the pertaining box –see fig 125. The animation can be started by pressing button labeled as *Replay*. Notice that geometric parameters have not been shown during optimization. You can chose them now, as indicated in section 4.2, to be displayed during animation. The starting geometry of the cluster can be restored by pressing *Reset* button.

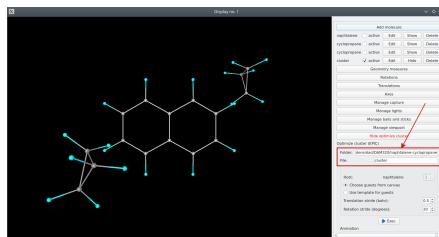


Figure 124: Setting file for animation

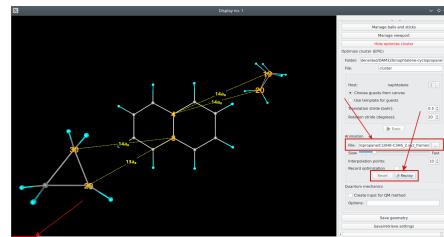


Figure 125: Starting animation

13. Animation can be recorded by checking the box labeled as *Record optimization* and pressing the *Replay* button. While recording is in progress, a message will appear as shown in fig 126

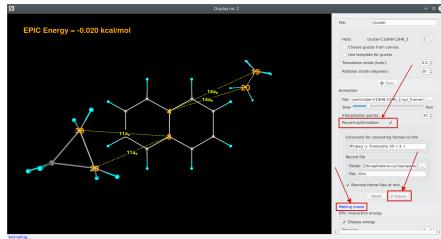


Figure 126: Recording animation

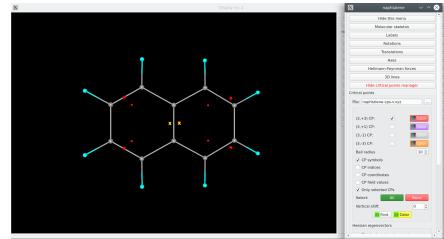


Figure 127: Cluster from MESP CPs

14. To generate the cluster from host MESP CPs and a guest template, execute steps 1–4, and load host MESP CPs from the corresponding *\*-cps-v.xyz* file. Select the CPs that you want to use as starting points by double clicking on them –see fig 127.
15. Add the molecule to be used as a template by loading its *.xyz* file. In this case it is neither necessary to add more than one guest molecule nor to displace them, as they will be created and placed according to the host MESP CPs.
16. Check the button labeled *Use template for guests* and, if only selected CPs are wanted as initial points, check the pertaining box too –see fig 128.

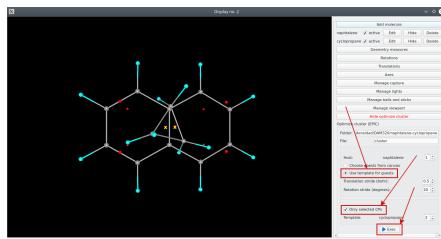


Figure 128: Working with selected MESP CPs

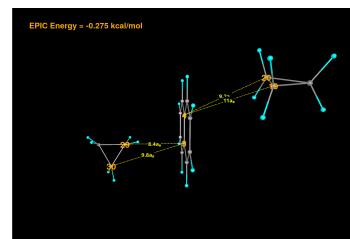


Figure 129: Translations and rotations during optimization

17. Push the *Exec* button to start optimization.
18. Notice that cluster can be translated or rotated while optimizing to change the viewpoint –see fig 129. These changes will be applied also when recording. In this regard, it is important to note that recording is made by capturing the pixels of the canvas. As a consequence, any change that may appear in the canvas while capturing (a popup message, for instance) will appear in the movie.

## G Appendix: Known issues

In MS-Windows some capture formats are not allowed, in particular this happens with JPG, JPEG and TIFF formats.

When 3D display editor is undocked, values in spinboxes can be changed only with the right arrows. All the features are restored when the menu is docked back.

## Credits and acknowledgments

DAMQT is an opensource project and, as such, it has profitted from the unselfish work of many other people involved in free software and opensource developments. Here we will explicitly acknowledge the most conspicuous but we want to extend our warmest recognition to all the people who have contributed in a variety of manners, from solving doubts to providing useful pieces of codes for some specific purposes. We thank ...

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OpenBabel, VLC and ffmpeg developers for their outstanding work and generosity offering their excellent products for free distribution and usage.

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