

User's Guide to DAMQT 3.2.0

Rafael López*, David Zorrilla[†] and Anmol Kumar[‡]

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*Universidad Autónoma de Madrid, Facultad de Ciencias. Departamento de Química Física Aplicada.

[†]Universidad de Cádiz, Facultad de Ciencias. Departamento de Química Física

[‡]Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur 208016, India

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DAMQT 3.2.0

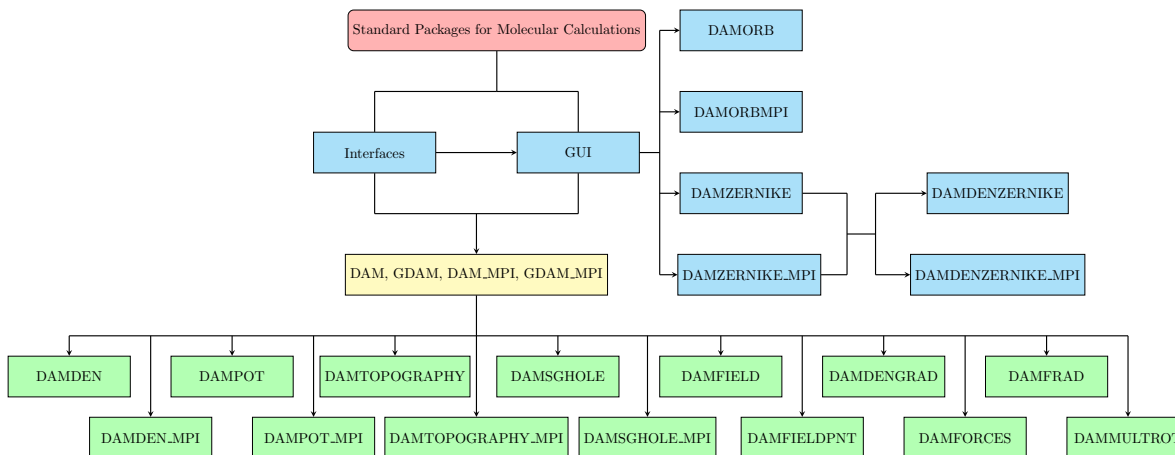
DAMQT is a package for the analysis and visualization of the molecular electron density (MED) in atoms and molecules, and several related properties like density deformations, electrostatic potential, molecular topography, sigma holes, electric field, Hellmann-Feynman forces, molecular orbitals and density fingerprints in Zernike-Canterakis and Jacobi functions.

The method used is based on the DAM partition of the electron density into atomic fragments by means of a least deformation criterion described elsewhere¹. 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 functions².

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, MOPAC and NWCHEM are currently included in the package, as well as a facility to read MOLEKEL *.mkl* files.



1

Figure 1: DAMQT structure

In this level too, DAMQT includes the GUI designed to facilitate usage. This GUI is written in C++ and has been developed using Qt library³, to facilitate portability between different operating systems. Also

¹For 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

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

³The Qt Company, www.qt.io

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.

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.

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 and a display area for applications standard outputs, and a menu on the right for handling graphical viewers (fig. 3).

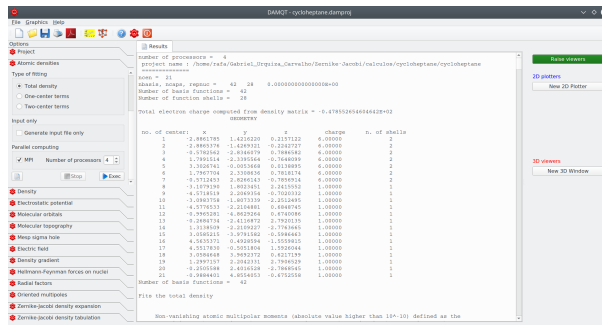


Figure 3: DAMQT main window

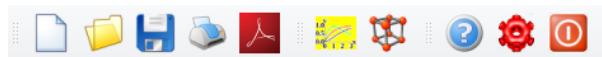












Figure 4: DAMQT toolbar

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
-  **2D viewer** Launch 2D viewer
-  **3D viewer** Launch 3D viewer
-  **Help** Show this help
-  **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* switches between 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 a LCAO calculation at any level of computation. One file is necessary in all cases with extension *.ggs* (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, ρ_{ij} , the extension in this case being *.densprsbm*.

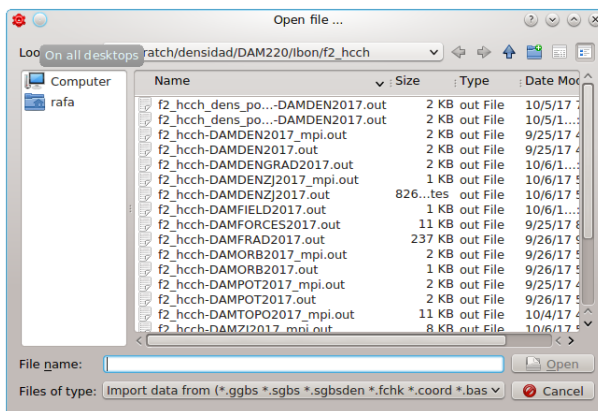



Figure 5: Import file navigator

Files *.ggs* (*.sgbs*) and *.den*, *.den.gz* or *.densprsbm* () can be loaded by supplying their full name (including path) in the box labeled *Import data from*. Alternatively, the name of a GAUSSIAN⁴ *.fchk* file, a MOLEKEL file *.mkl*, a TURBOMOLE basis set or coords file *.basis*, *.coords*, a MOLPRO output file, *.out*, or *.xml* file, a NWCHEM output file, *.nwcout*, or a MOPAC *.aux* file can be supplied. In each case, a suitable built-in interface included in the package will automatically generate the *.ggs* 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.

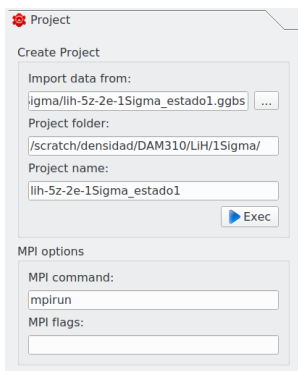


Figure 6: Project

Table 1: Suitable file extensions for running interfaces

interface	extensions
GAUSSIAN	*.fchk
MOLEKEL	*.mkl
MOLPRO	*.out, *.xml
MOPAC	*.aux
NWCHEM	*.nwcout
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 *.ggb*s 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 temptatively will assign a name to the project equal to that of the *.ggb*s 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.

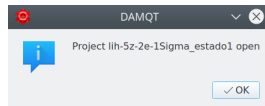
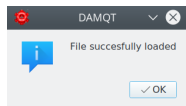




Figure 7: Project upload Figure 8: Project opening

If an existing *.ggb*s 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 *.ggb*s (*.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.

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.

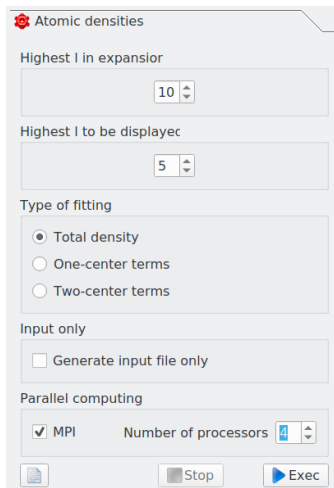



Figure 9: Atomic densities menu

⁴www.gaussian.com

The following options can be set:

- *Highest l in expansion:* defines the order of the multipolar 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.
- *Input only:* 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.

The key  must be pressed to compute the expansion. Besides the `_2016.damqt`, a file, whose name ends in `_2016.damqtv` 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.

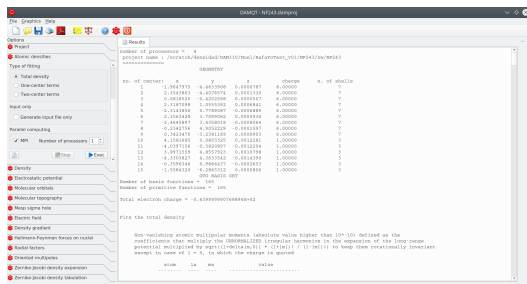


Figure 10: Standard output

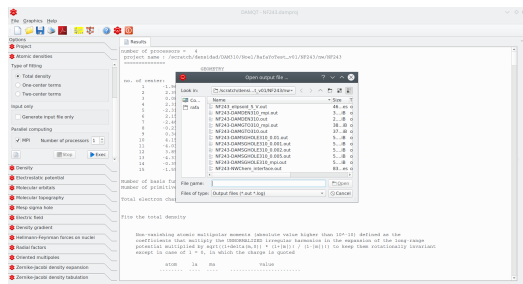




Figure 11: Standard output files menu

Another file with extension *.mltmod* containing the modules 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 modules 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 multipolar expansion up to the desired order. When the *Highest l* is equal 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, 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. 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.

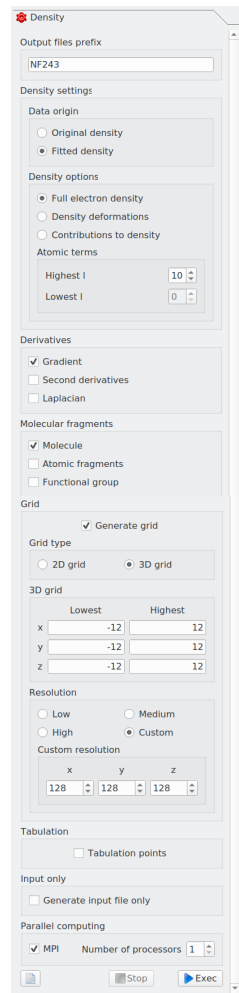


Figure 12: Density menu

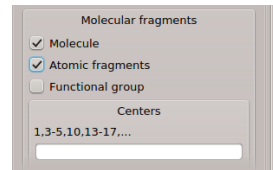


Figure 13: Single atom densities

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.

Figure 14: 2D Grid settings

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 gOpenMol⁵. For systems with *mpi* installed, parallel computing can be chosen as in case of *Atomic densities*.

Figure 15: 3D Grid settings

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?.cnt: 2D grid tabulation files with first derivatives ($?$: x, y, z).

\$fname-d???.cnt: 2D grid tabulation files with second derivatives ($??$: xx, xy, \dots, 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-?.pltd*: 3D grid tabulation files with first derivatives of density or deformations ($?$: x, y, z).

\$fname--d-???.pltd*: 3D grid tabulation files with second derivatives of density or deformations ($??$: xx, xy, \dots, 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 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, 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 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?.pltd*, 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.

Figure 16: Electrostatic potential

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.

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.

⁵www.csc.fi/gopenmol/

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.

Molecular orbitals

Molecular orbitals

Import data from:

Output files prefix
cycloheptane

Molecular orbitals
1.3-5.10.13-17,...
1

Derivatives
☐ Gradient

Grid
☒ Generate grid

Grid type
☐ 2D grid ☒ 3D grid

3D grid
Lowest Highest
x -4 4
y -4 4
z -4 4

Resolution
☐ Low ☐ Medium
☐ High ☒ Custom

Custom resolution
x y z
64 64 64

Input only
☐ Generate input file only

Parallel computing
☒ MPI Number of processors 1

Stop Exec

Figure 17: Molecular orbitals

Molecular topography

Output files prefix
f2_hcch

Topography type
☐ Molecular density
☒ Molecular potential
Highest l in expansion 10

Topography mapping
☒ Map critical points
Box margins size 1.0
Convergence threshold 4.0e-12
☒ Add guess points for CPs
☒ Add guess points to table

x	y	z
1	-6.8	

Load guess points from file
hcch/f2_hcch_extra_cps.xyz

Box size 5.0
Step size 0.2

☐ Construct molecular graph
☐ Construct atomic basin

Input only
☐ Generate input file only

Parallel computing
☒ MPI Number of processors 1

Stop Exec

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.gpd* or *\$fname-v.gpd*. In case of atomic basin, 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 bohr²) 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 then this threshold), for MESP long-range (short-range contributions are not computed when they are lower than it), and for local extrema. MESP is computed from the DAM expansion of density.

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 4.9.7– 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 ν parameter, introduced by P. Politzer, J.S. Murray et al.⁶

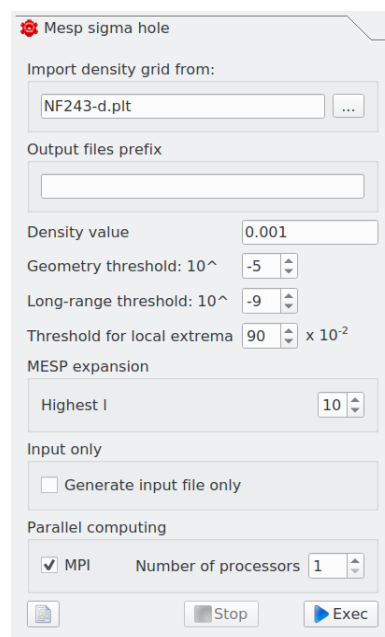


Figure 19: MESP sigma hole

⁶P.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)

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.

2.8 Electric field

Tab *Electric field* manages the module for the computation of electric field lines from the atomic multipolar 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 stepsize 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 employed for defining 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*.

Electric field

Output files prefix:

Highest l in expansion:

Long-range: ☐ Long-range only
Long-range threshold: 10^{-4}

Lines
Highest number of points:
Stride length:

Plot type
☒ 2D grid ☐ 3D grid

2D Plot
Number of lines per nucleus:
Lowest Highest
u:
v:
2D Planes
☐ XY ☐ XZ
☒ YZ ☐ Other

☒ Extra lines

☒ Add starting points to table

	cntr	u	v
1		-6	15
2		6	15
3		-0.01	12.9
4		0.01	12.9
5		0	15

Read from file:

Figure 20: Electric field

Density gradient

Output files prefix:

Highest l in expansion:

Long-range: ☐ Long-range only
Long-range threshold: 10^{-9}

Lines
Highest number of points:
Stride length:

Plot type
☒ 2D grid ☐ 3D grid

2D Plot
Number of lines per nucleus:
Lowest Highest
u:
v:
2D Planes
☐ XY ☐ XZ
☒ YZ ☐ Other

☒ Extra lines

☒ Add starting points to table

	cntr	u	v
1		0	-6.9

Read from file:

Figure 21: Density gradient

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 multipolar 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 topology* 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 corresponds 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 conditions⁷)*. 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.

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*.

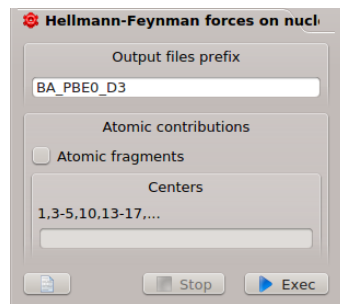


Figure 22: H-F forces

Besides these files, detailed information about the electrostatic potential, electric field and forces on the nuclei is given in the standard output (main panel).

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.

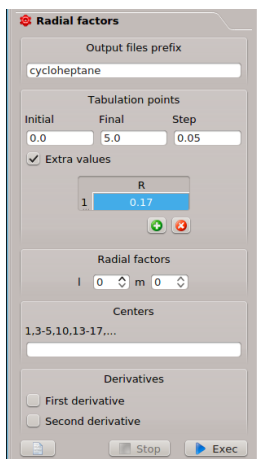


Figure 23: Radial factors

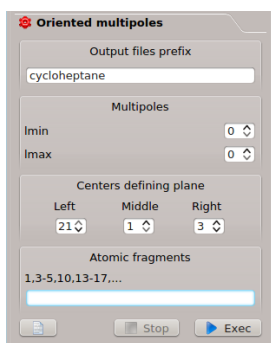


Figure 24: Oriented multipoles menu

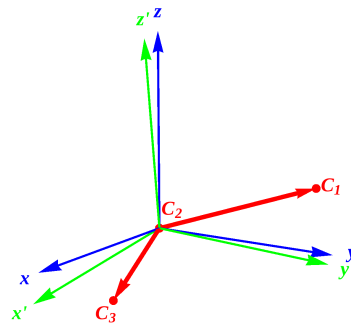


Figure 25: Oriented multipoles frame

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 multipolar 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 $\widehat{C_1 C_2 C_3}$ (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

⁷Berlin T J Chem Phys 19 (1951) 208

expansion coefficients, Ω_{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 Ω_{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.

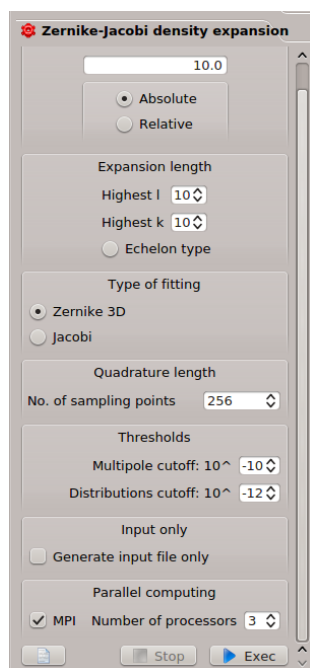


Figure 26: Zernike-Jacobi expansion

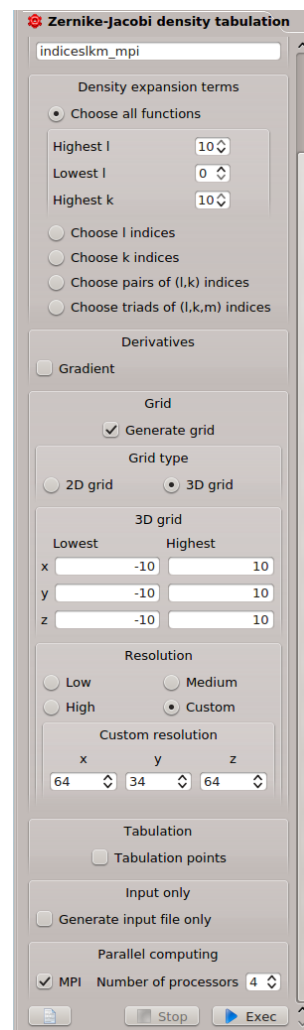


Figure 27: Zernike-Jacobi tabulation

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 length 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 user can also set the size of this quadrature.

The screenshot shows the 'Zernike-Jacobi density tabulation' window. Under 'Density expansion terms', the 'Choose l indices' radio button is selected. The 'Select indices' field contains '0,3-5,7'. Other options like 'Choose all functions', 'Choose k indices', 'Choose pairs of (l,k) indices', and 'Choose triads of (l,k,m) indices' are unselected. The 'Derivatives' section has 'Gradient' unchecked. The 'Grid' section has 'Generate grid' checked and '3D grid' selected. The '3D grid' section shows ranges for x, y, and z from -10 to 10. The 'Resolution' section has 'Custom' selected. The 'Custom resolution' section shows x, y, and z values of 64, 34, and 64 respectively. The 'Tabulation' section has 'Tabulation points' unchecked. The 'Input only' section has 'Generate input file only' unchecked. The 'Parallel computing' section has 'MPI' checked and 'Number of processors' set to 4.

Figure 28: Choose l option

The screenshot shows the 'Zernike-Jacobi density tabulation' window. Under 'Density expansion terms', the 'Choose pairs of (l,k) indices' radio button is selected. The 'Select pairs of indices' field contains '(0,0),(1,0),(1,1),(2,0)'. Other options are unselected. The 'Derivatives' section has 'Gradient' unchecked. The 'Grid' section has 'Generate grid' checked and '3D grid' selected. The '3D grid' section shows ranges for x, y, and z from -10 to 10. The 'Resolution' section has 'Custom' selected. The 'Custom resolution' section shows x, y, and z values of 64, 34, and 64 respectively. The 'Tabulation' section has 'Tabulation points' unchecked. The 'Input only' section has 'Generate input file only' unchecked. The 'Parallel computing' section has 'MPI' checked and 'Number of processors' set to 4.

Figure 29: Choose (l, k) option

The screenshot shows the 'Zernike-Jacobi density tabulation' window. Under 'Density expansion terms', the 'Choose triads of (l,k,m) indices' radio button is selected. The 'Select triads of indices' field contains '(0,0,0),(1,0,-1),(1,0,0)'. Other options are unselected. The 'Derivatives' section has 'Gradient' unchecked. The 'Grid' section has 'Generate grid' checked and '3D grid' selected. The '3D grid' section shows ranges for x, y, and z from -10 to 10. The 'Resolution' section has 'Custom' selected. The 'Custom resolution' section shows x, y, and z values of 64, 34, and 64 respectively. The 'Tabulation' section has 'Tabulation points' unchecked. The 'Input only' section has 'Generate input file only' unchecked. The 'Parallel computing' section has 'MPI' checked and 'Number of processors' set to 4.

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 chosen, 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 29). 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 [29](#) and [30](#)). In these cases, parenthesis are just optional cosmetic aids to help in identifying pairs of 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.

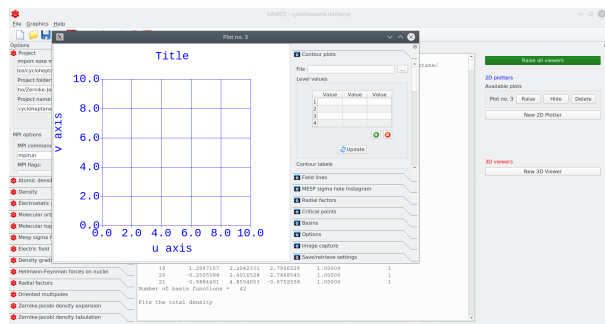



Figure 31: 2D viewer window

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.

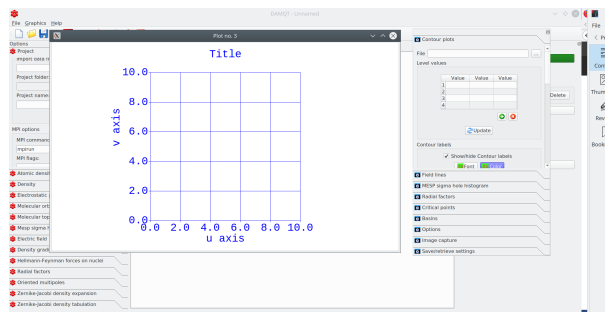


Figure 32: 2D viewer: undocked menu

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

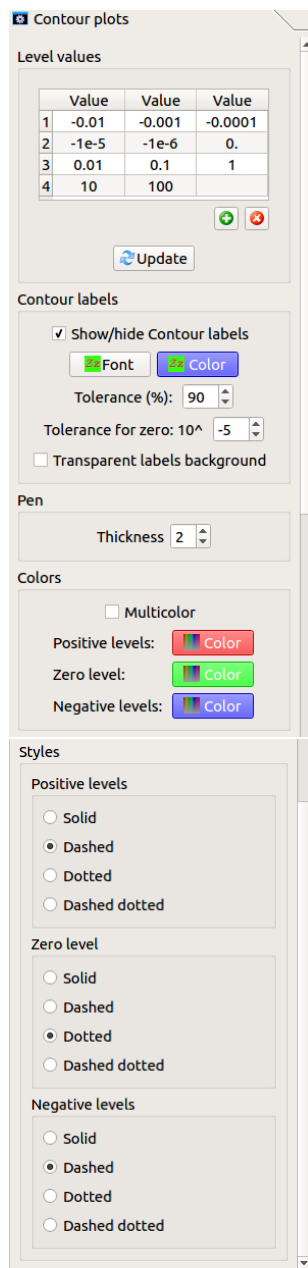


Figure 33: Contour plots

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 *OYZ* 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).

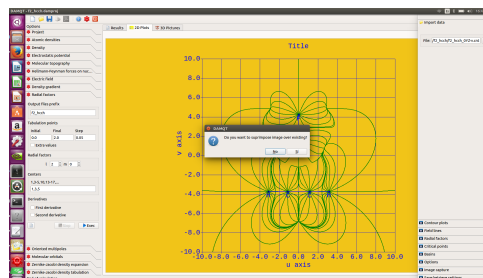


Figure 34: Combining plots

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.

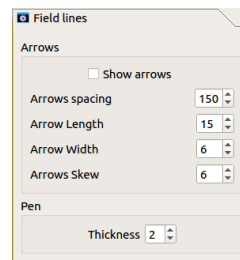


Figure 35: Field lines

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).

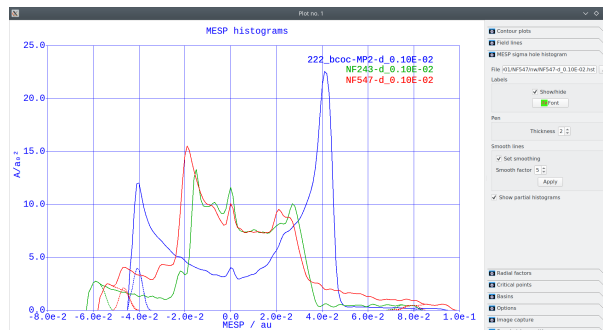


Figure 36: MESP sigma hole histogram

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)

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.

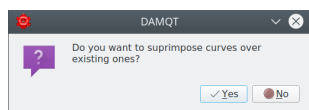


Figure 37: Adding curve to current plot

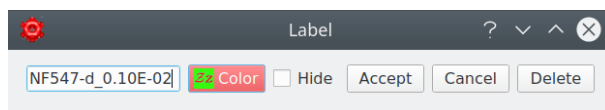


Figure 38: Histogram curve editor

Labels can be dragged by keeping the **Shift** key and the *Left* mouse button pressed 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*.

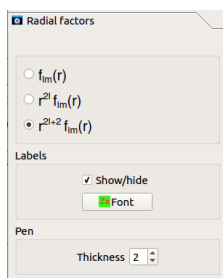


Figure 39: Radial factors

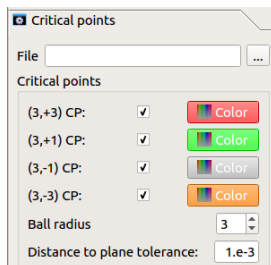


Figure 40: Critical points

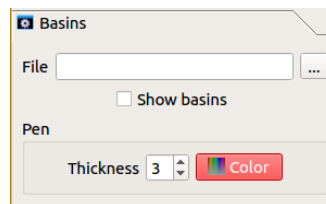


Figure 41: Atomic basins

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.

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.

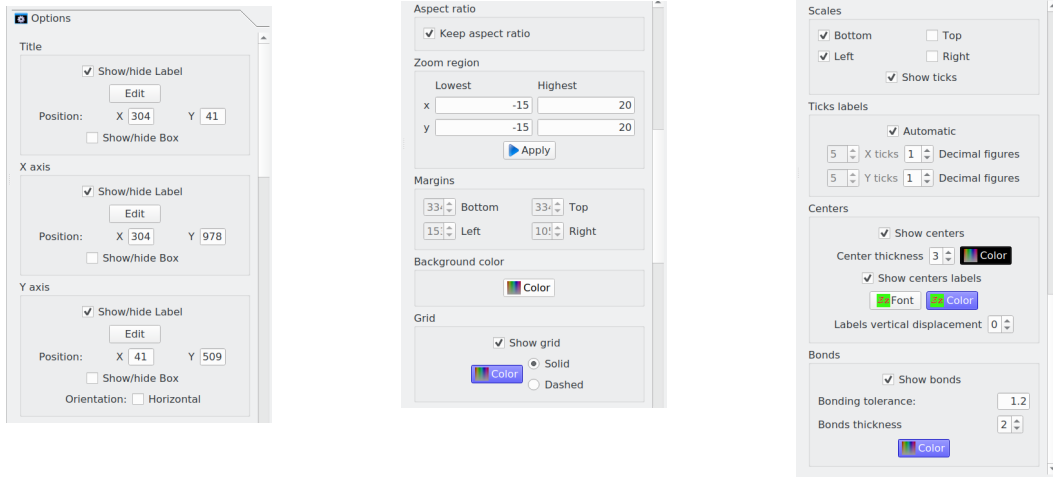


Figure 42: Options

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).

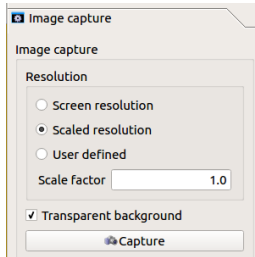


Figure 43: Image capture

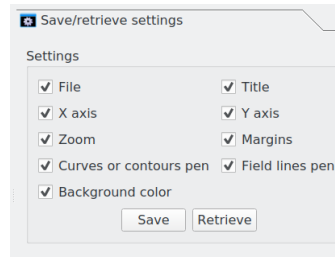


Figure 44: Save/retrieve

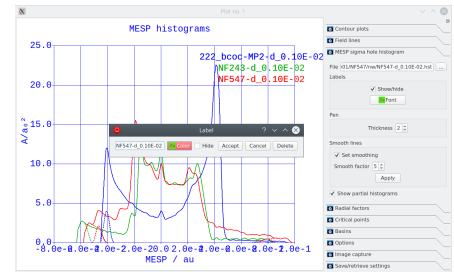


Figure 45: Sigma hole histogram popup window

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).

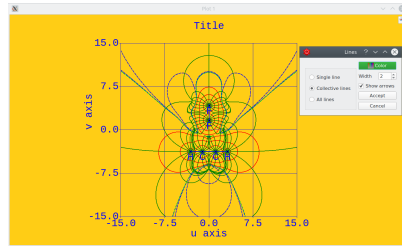


Figure 46: Field lines popup window

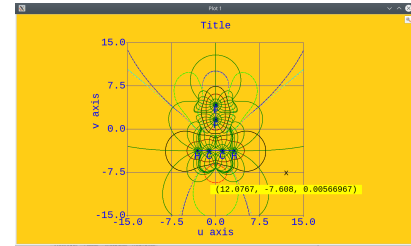





Figure 47: Point coordinates and value

- 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 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* \rightarrow *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 eight items: *Add molecule*, *Geometry measures*, *Manage capture*, *Record animation*, *Manage lights*, *Manage balls and sticks*, *Manage viewport* 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.

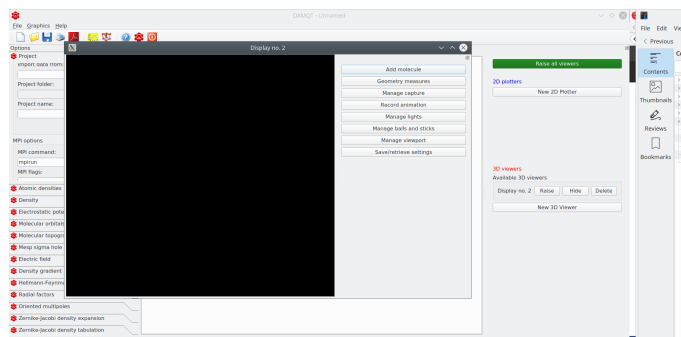


Figure 48: 3D viewer

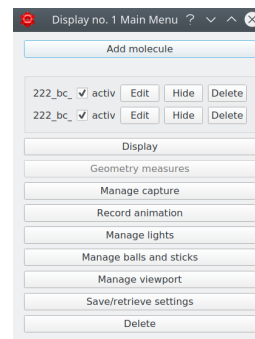


Figure 49: 3D menu with two molecules loaded

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 *.ggs*, *.sgbs* and *.xyz*. Furthermore, geometry can be loaded from any text file with the following format:

NCEN

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 *.ggs* file, whereas they are given in Angstrom in file *.xyz*; this is so for compatibility of *.xyz* files with gOpenMol and other packages. Notice the blank line after NCEN.

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 below. Rotation and translation

operations will be performed only on molecules whose boxes are checked (active). Activation can be toggled also by double clicking on a molecule structure while holding the **Ctrl** key pressed.

Active molecules can be rotated around the x and y axes 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.

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.

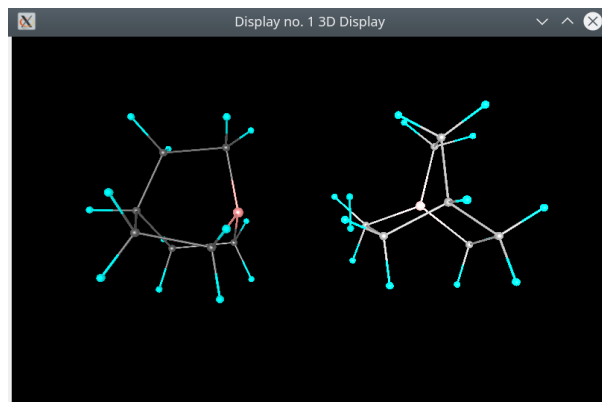


Figure 50: 3D display

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.

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

4.2 Geometry measures

Use the *Geometry measures* button to measure distances, angles and dihedral angles between atomic centers or critical points of a molecule. 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.

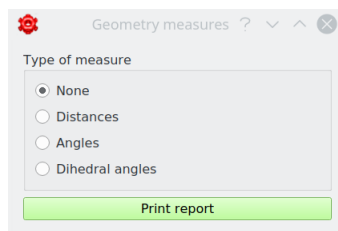


Figure 51: Measures window

To measure a distance between a pair of centers, the *Distances* button must be checked, and the pairs of centers are chosen by pressing the **Shift** key while double clicking on them in the display. 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. In this case, when more than one molecule has been

loaded in the viewer, the pairs of centers are collected within parenthesis with a subscript indicating the molecule order index.

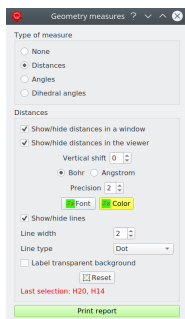


Figure 52: Distances menu

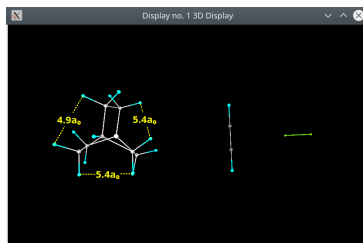


Figure 53: Distances display



Figure 54: Distances window

To measure the angle between three centers, the *Angles* button must be checked, and the centers are chosen by pressing the **Shift** key while double clicking on them in the display. 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. In this case, when more than one molecule has been loaded in the viewer, the triads of centers are collected within parenthesis with a subscript indicating the molecule index.

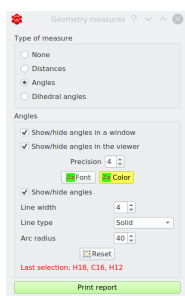


Figure 55: Angles menu

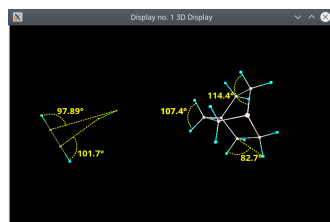


Figure 56: Angles display



Figure 57: Angles window

To measure the dihedral angle between four centers, the *Dihedral angles* button must be checked, and the centers are chosen by pressing the **Shift** key while double clicking on them in the display. The first three centers define one plane and the second plane is defined by centers 1, 2, 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. In this case, when more than one molecule has been loaded in the viewer, the tetrads of centers are collected within parenthesis with a subscript indicating the molecule order index.

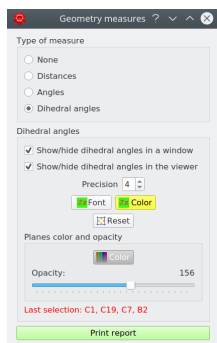


Figure 58: Dihedral angles menu

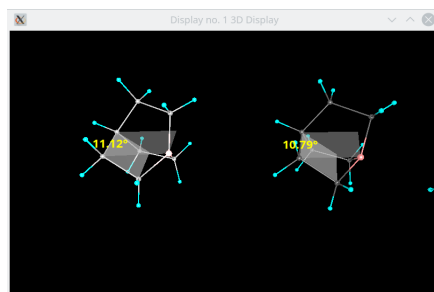


Figure 59: Dihedral angles display

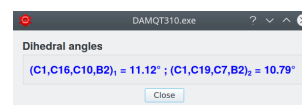


Figure 60: Dihedral angles window

4.3 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 61. 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.

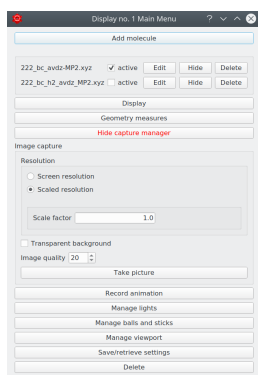


Figure 61: Image capture

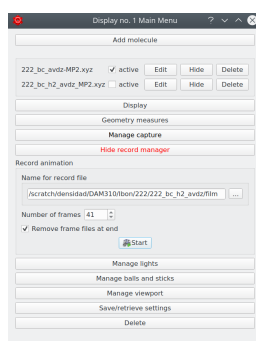


Figure 62: Animation record

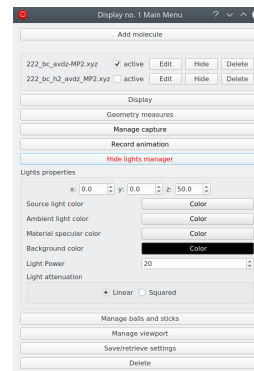


Figure 63: Lights

4.4 Record animation

The *Record animation* button displays a menu for recording frames of the 3D viewer content upon rotation of any of the molecules –see fig 62. It must be used in combination with the *Rotations* options of the molecule editor -see section 4.9.4. 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.

4.5 Lights manager

The *Manage lights* button displays a menu for lighting options, including background color –see fig 63. 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.

4.6 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 64.

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.

4.7 Viewport manager

The *Manage viewport* button displays a menu with options for viewport –see fig 65– including *Far* and *Near* clipping planes.

Clipping planes can be used to get slices of 3D images –see fig 67. 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 4.9.4– 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 4.9.9.

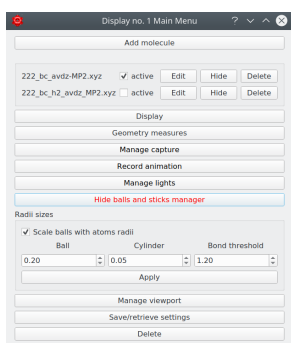


Figure 64: Balls and sticks

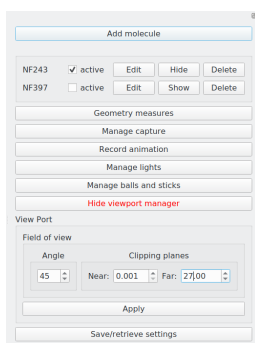


Figure 65: Viewport

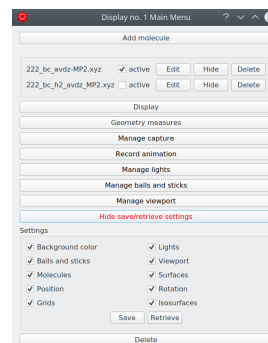


Figure 66: Save/retrieve

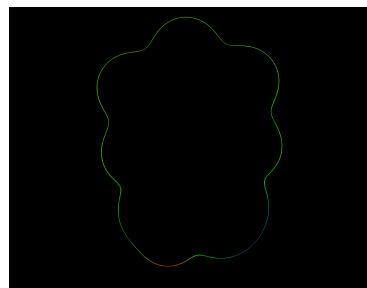
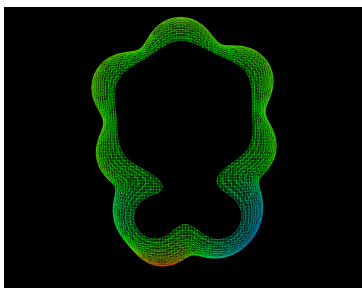
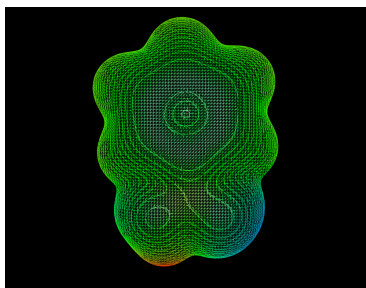


Figure 67: 3D surface slices

4.8 Save/retrieve settings

The *Save/retrieve settings* button saves the current settings of the image display or retrieves settings previously saved –see fig 66. Files with settings have extension *.3Dsettings*.

4.9 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 68. Acceptation causes the corresponding molecule and all properties related to it (structure, surfaces, critical points, field lines, etc) to be removed from the viewer.

The *Edit* button opens a window with a menu for editing the molecule as shown in fig 69. Eight options for edition appear in the menu: *Molecular skeleton*, *Labels*, *Rotations*, *Translations*, *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.

4.9.1 Molecular skeleton

Pressing the *Molecular skeleton* button, a menu like that shown in fig 70 is displayed in the editor to show/hide atoms, bonds or hydrogens in the structure.

4.9.2 Labels

Pressing the *Labels* button, a menu for handling atom labels is displayed –see fig 71. 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 72. 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 73. 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.

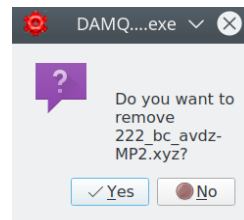


Figure 68: Delete molecule confirmation

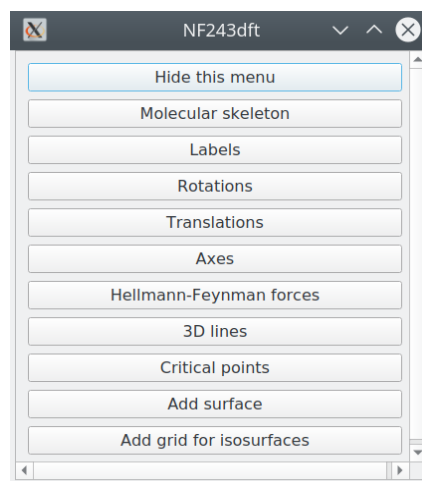


Figure 69: Molecule editor

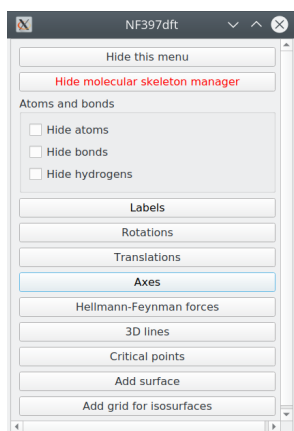


Figure 70: Molecular skeleton

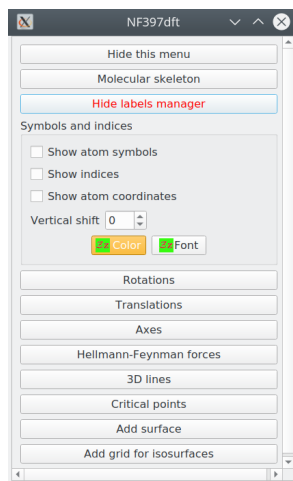


Figure 71: Atom labels

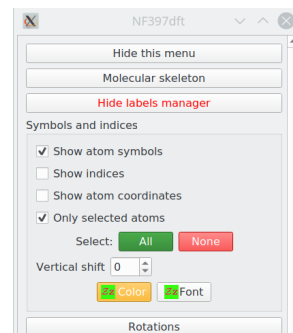


Figure 72: Select atoms

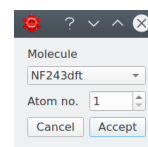


Figure 73: Selection menu

4.9.3 Rotations

The *Rotations* button opens a menu for rotation manager –see fig 74. 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 4.5 to capture frames and making movies. In this case, animation ends when recording finishes.

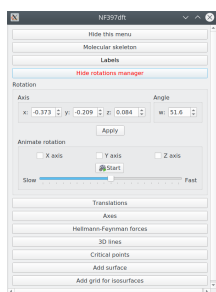


Figure 74: Rotations menu

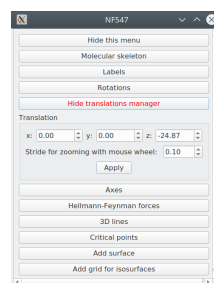


Figure 75: Translations menu

4.9.4 Translations

The *Translations* button opens a menu for translation manager –see fig 75. 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.

4.9.5 Axes

The *Axes* button opens a menu for molecular axes manager –see fig 76.

4.9.6 Hellmann-Feynman forces

The *Hellmann-Feynman forces* button opens a menu for displaying Hellmann-Feynman forces on nuclei –see fig 77. H-F forces are computed with the pertaining module of right menu –see 2.10– and stored in *.forces* files.

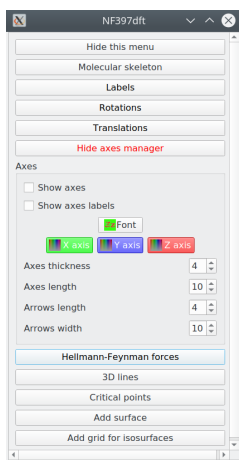


Figure 76: Molecular axes menu

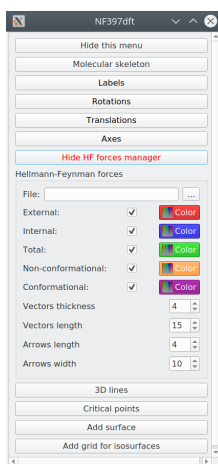


Figure 77: HF forces menu

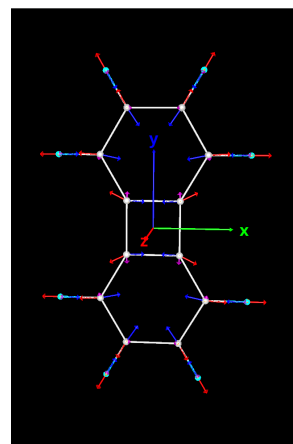


Figure 78: HF forces and molecular axes

4.9.7 3D lines

The *3D lines* button displays a menu for loading and managing lines in space –see fig 79– 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 80– by checking the appropriate box in the menu.

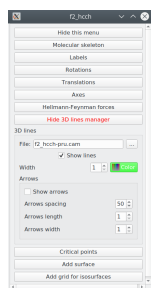


Figure 79: Field lines menu

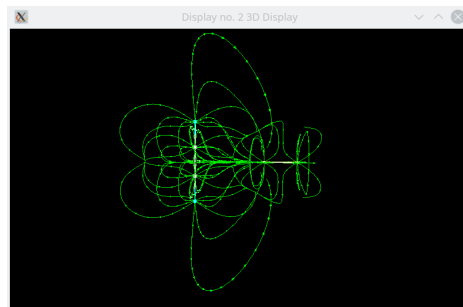


Figure 80: Field lines display

4.9.8 Critical points

The *Critical points* button displays a menu for loading and managing MED or MESP critical points –see fig 81. File names are ended in *-cps-d.xyz* for MED CPs, and *-cps-v.xyz* for MESP CPs.

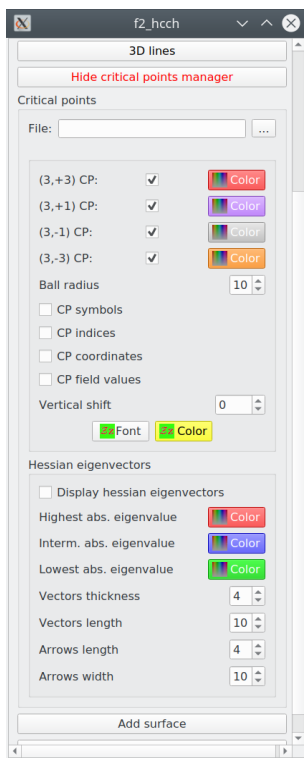


Figure 81: Critical points menu

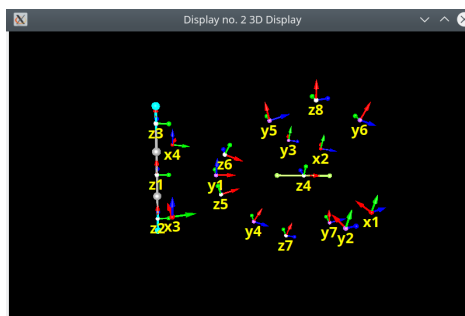


Figure 82: Hessian eigenvectors at critical points

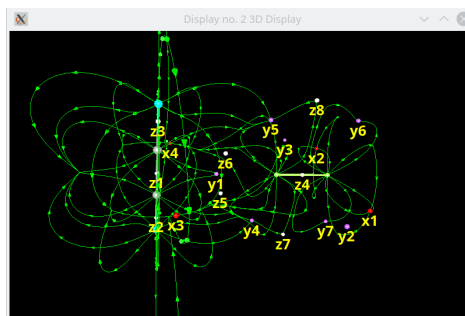


Figure 83: Critical points and field lines

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 81). 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 83.

4.9.9 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*, and MED or MESP basins borders, with extension *.basins* can be visualized.

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 84. If the *Edit* button is pressed, a menu is displayed whose content depends on whether basins borders –see fig 85– or sigma hole surfaces are loaded –see fig 86. The button label changes to *Close* and, if pressed again, all the surfaces menus are closed.

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

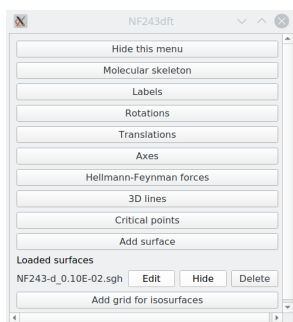


Figure 84: Surfaces menu

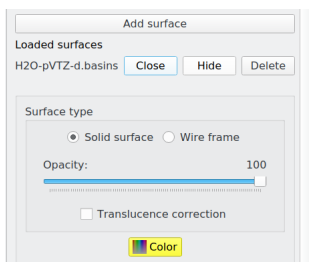


Figure 85: Basins options

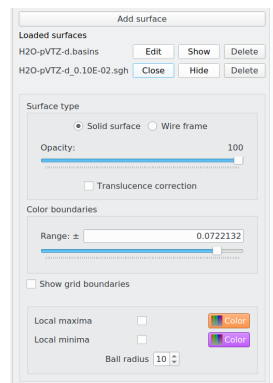


Figure 86: Sigma hole options

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 88.

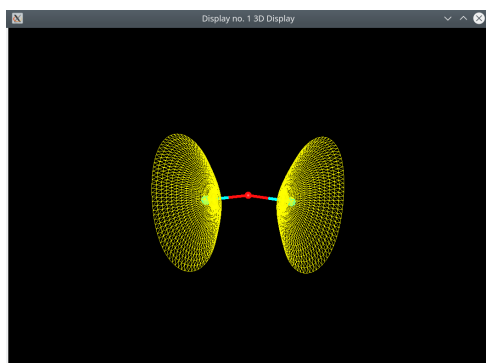


Figure 87: Basins borders

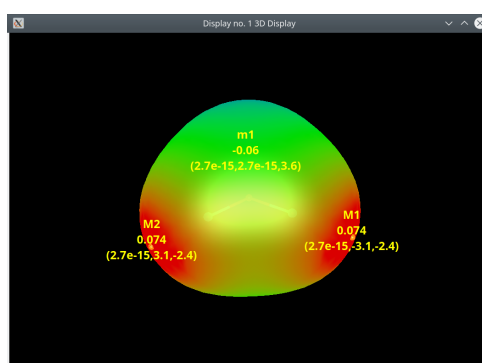


Figure 88: Sigma hole surface

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.

4.9.10 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*.

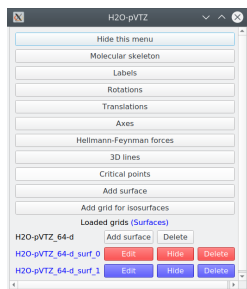


Figure 89: Basins borders

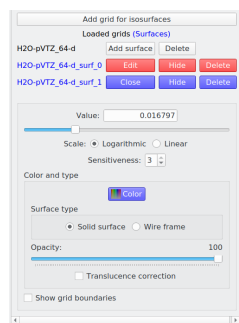


Figure 90: Sigma hole surface

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 89– 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 90.

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 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.

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

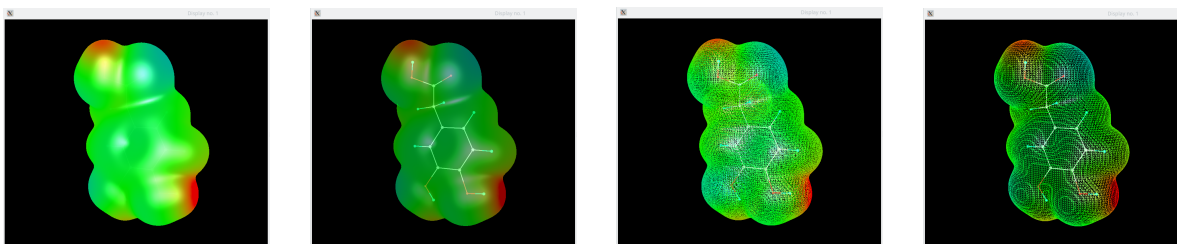


Figure 91: Surface display modes. From left to right: solid, solid with transparency, wired, wired with transparency and translucency correction.

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 91.

4.10 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, and vertical displacements, rotation around the space-fixed *x* axis.
- Holding the *right button*, mouse displacements cause rotation around the space-fixed *z* axis.
- 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.
- 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 4.9.2.
- 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 4.9.6.
- 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 4.9.7.
- 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 92 and 93. Accepting the action has the same effect as clicking directly on the nucleus or critical point.

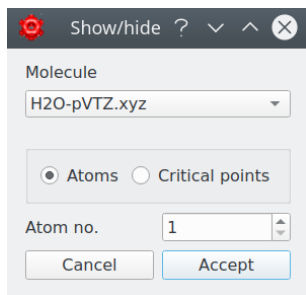


Figure 92: Atom selection

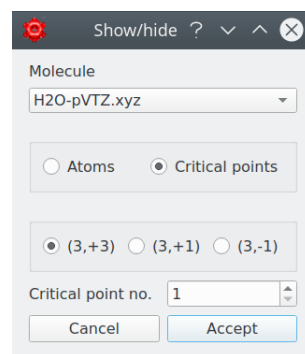


Figure 93: CP selection

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 *.gbs* 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 calculations are different in *.out* file from those of *.xml* file. In *.out* file 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.

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. It is recommended to give a common name to these files, which 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* .

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.

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 sets⁸. 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 94 shows the total density of CH₃Cl (left plate) and the density corresponding to only spherical atomic terms (right plate).



Figure 94: Electron density of CH₃Cl. *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 95 shows some density deformation contours for CH₃Cl.



Figure 95: Density deformations of CH₃Cl. *Left*: positive deformations (charge accumulation), *right*: negative deformations (charge depletion). Contour values: ± 0.08 , ± 0.04 , ± 0.02 , ± 0.01

⁸cita a Dunning

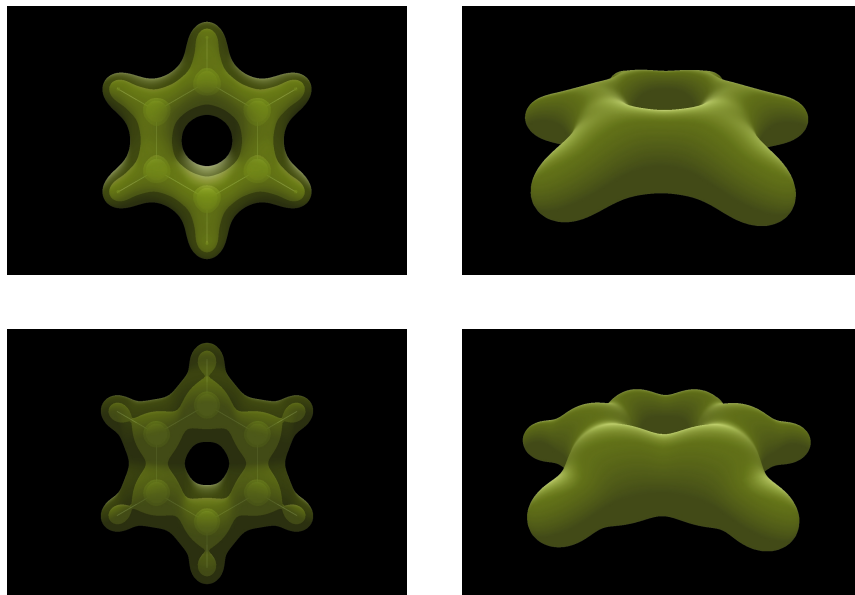


Figure 96: Electron density of C_6H_6 . *Upper*: full density. *Lower*: only atomic spherical terms. Contour values: 0.8, 0.3, 0.2, 0.1 (only 0.1 in right plates).

Figures 96 and 97 show some contour density and density deformations surfaces for benzene.

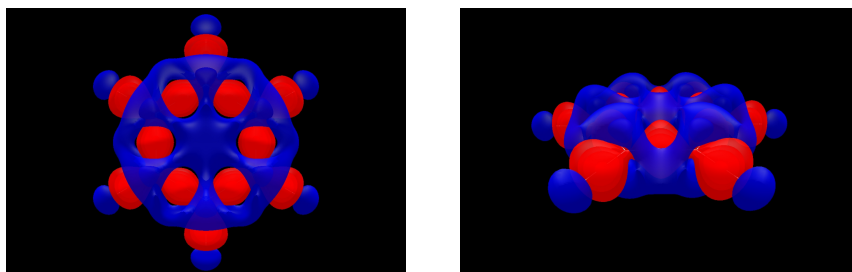


Figure 97: Density deformations of C_6H_6 . *Red*: positive deformations (charge accumulation), *blue*: negative deformations (charge depletion). Contour values: 0.09, 0.05, ± 0.03 , ± 0.01

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 98 and 99 show the full atomic density and its related deformations for chlorine and carbon atoms in CH_3Cl .



Figure 98: Atomic density of Cl in CH_3Cl . *Left*: electron density, contour values: 20, 1, 0.2, 0.04; *right*: deformation, contour values: 0.1, 0.02, ± 0.01 , ± 0.005



Figure 99: Atomic density of C in CH_3Cl . *Left*: electron density, contour values: 5, 1, 0.2, 0.04; *right*: deformation, contour values: 0.05, 0.02, ± 0.01 , ± 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.

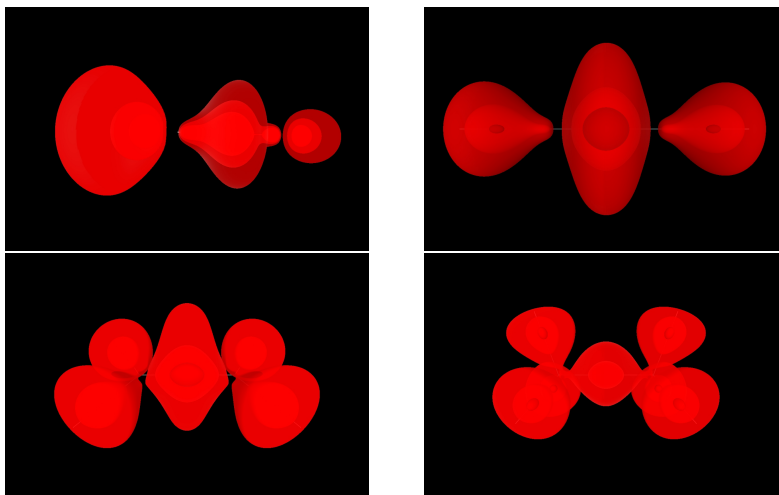


Figure 100: Positive density deformations (charge accumulation) *Upper left*: CO, *upper right*: C_2H_2 , *lower left*: C_2H_4 , *lower right*: C_2H_6 . Contour values: 0.09, 0.05, 0.01.

Figure 100 shows the charge accumulation (positive deformation) in four molecules containing carbon

with different bond types. Figure 101 shows the deformation pattern in CO and C₂H₂ including contours of charge depletion (negative deformation).

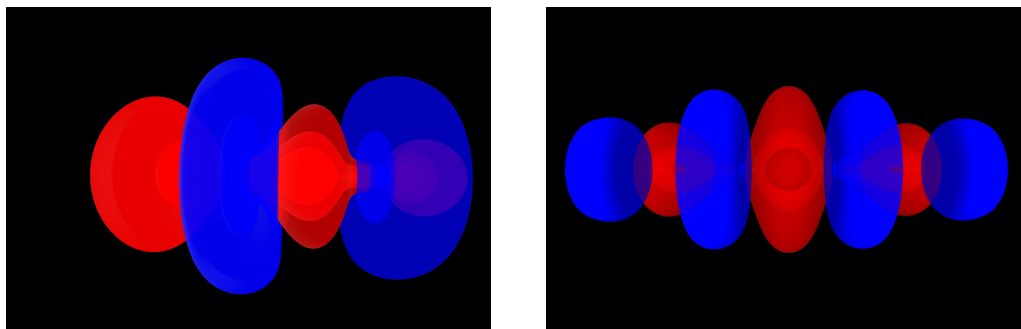


Figure 101: Density deformations (charge accumulation) in CO (*left*) and acetylene (*right*). Contour values: 0.09, 0.05, ± 0.01 .

In conjugated systems, it is also interesting to look at the deformations corresponding to contour values lower than those considered so far. Figure 102 shows the positive density deformation (charge accumulation) in C₆H₆ at low contour values. These plots correspond to high resolution grids (257x257x257) of a RHF density computed with Dunning's cc-pVQZ basis set.

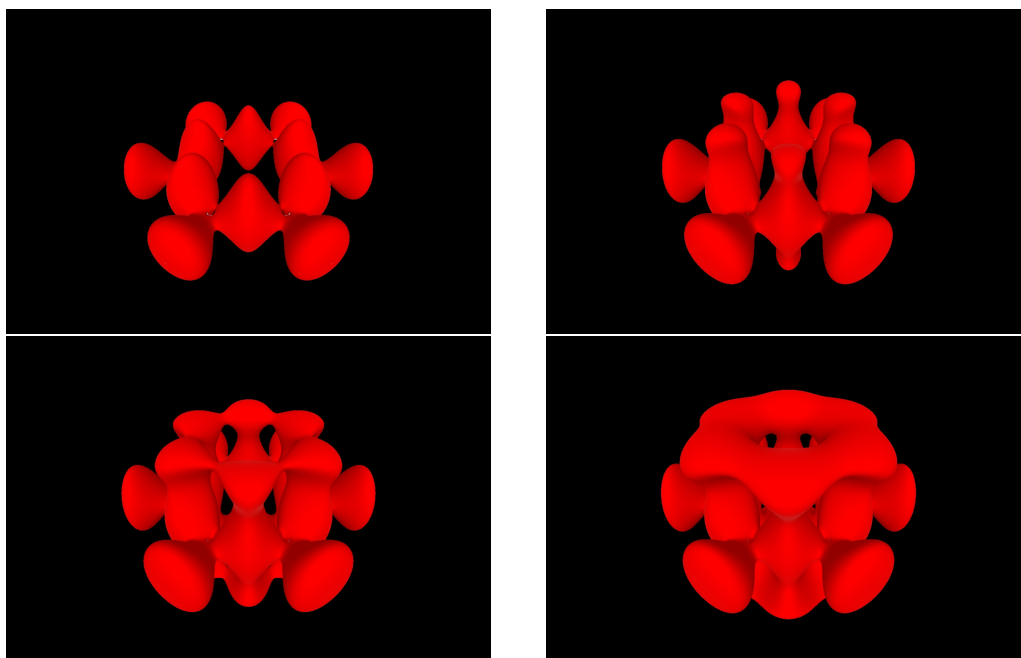


Figure 102: Positive density deformations (charge accumulation) in C₆H₆. Contour values: 0.005, 0.002, 0.0015, 0.001.

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 103 shows some electrostatic

potential contours of H_2O and NH_3 in the regions of negative (blue) and positive (red) potential values drawn from a high resolution grid ($257 \times 257 \times 257$). Positive and negative regions are separately plotted for CH_3Cl in figure 104.



Figure 103: Electrostatic potential of H_2O (*left*) and NH_3 (*right*). Contours: *red*: 15, 2, 1, 0.5, *blue*: -0.085, -0.080.



Figure 104: Electrostatic potential of CH_3Cl . *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 105 shows MESP critical points of H_2O and 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.

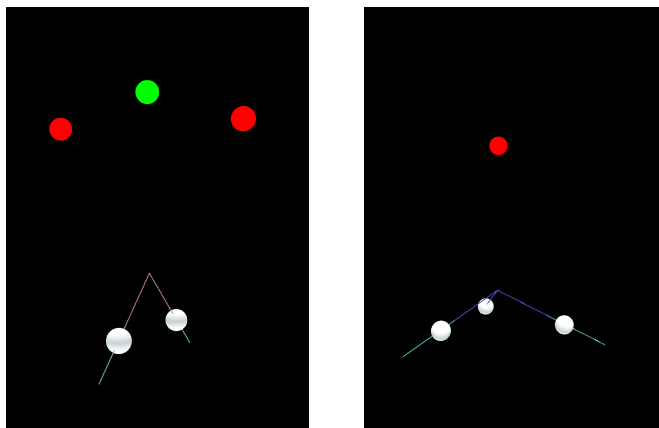


Figure 105: MESP critical points of H₂O (*left*) and NH₃ (*right*). (3,+3) CP: *red*; (3,+1) CP: *green*; (3,-1) CP: *grey*.

Figure 106 shows MESP-based topographs of H₂O and NH₃. These gradient field lines connecting various critical points and nuclei are constructed in the directions of maximum change of potential.

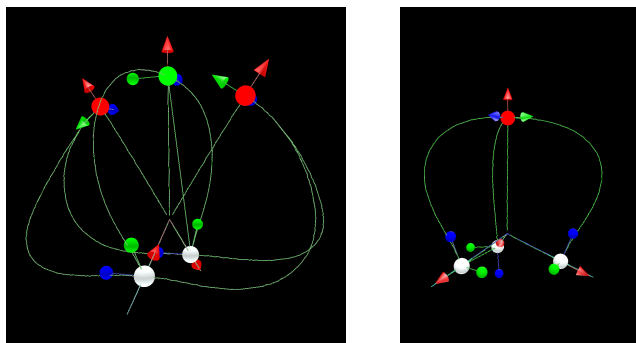


Figure 106: MESP-based topographs of H₂O (*left*) and NH₃ (*right*). Eigenvectors show the direction of maximum change of function value at the critical points.

Figure 107 shows MESP atomic basins of H₂O and NH₃. The oxygen atom in H₂O and nitrogen atom in NH₃ possess closed zero flux surfaces, whereas the hydrogens show open surfaces.

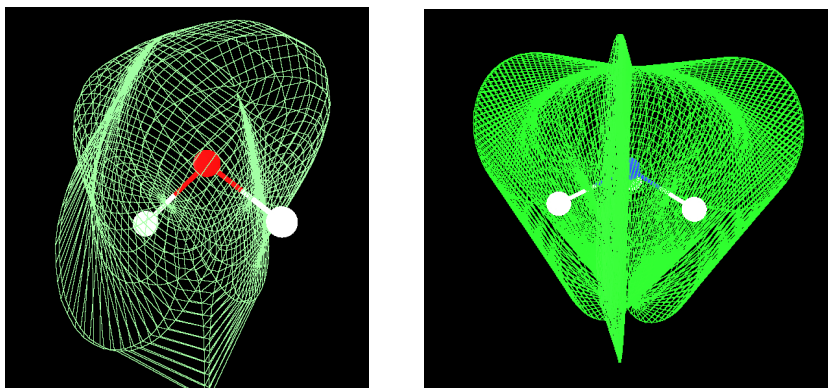


Figure 107: MESP-based atomic basins of H_2O (*left*) and NH_3 (*right*).

6.6 MESP sigma hole

MESP sigma hole can be computed over a MED isosurface of user-defined density value. Figure 108 shows the MESP sigma hole of benzoic acid over the MED isosurface of density 0.001 bohr^{-3} . The MESP maximum (over the acid proton) and the minimum are displayed together with their MESP values.

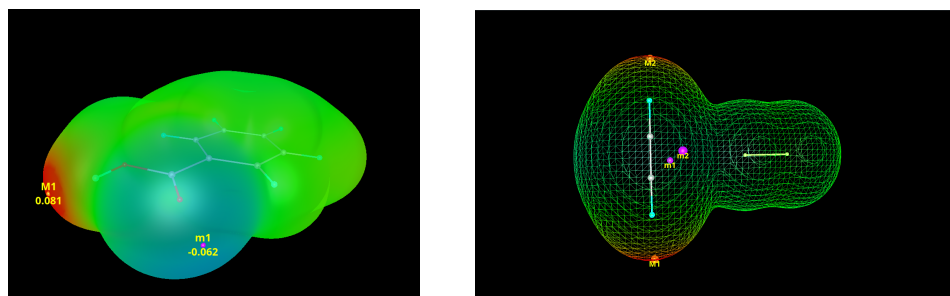


Figure 108: MESP extrema on sigma hole of Benzoic acid (*left*) and system HCCH-F_2 (*right*)

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 109 shows two different views of the field lines of H_2O .

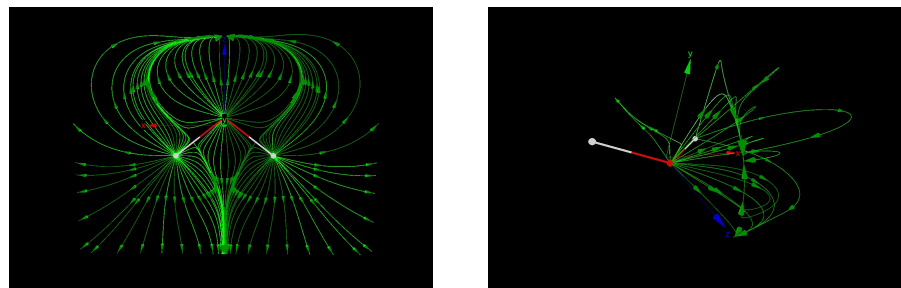


Figure 109: Electric field lines in H_2O

Relationship between the different types of MESP critical points and electric field lines is clearly shown in fig 110.

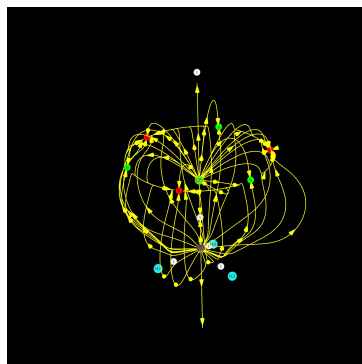


Figure 110: MESP CPs of CH_3Cl and electric field lines starting from carbon and chlorine.

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 111 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.

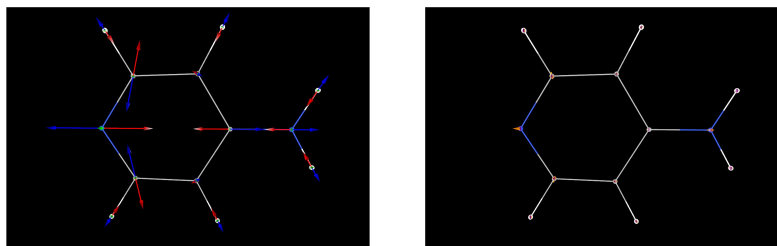


Figure 111: Hellmann-Feynman forces in 4-amine pyridine. *Left*: Internal (*red*), external (*blue*) and total (*green*) forces. *Right*: conformational (*orange*) and non-conformational (*purple*) forces.

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 Zernie-Canterakis functions as well as Jacobi functions of MED. Upper left panel of figure 112 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 remaning panels. A 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 113 for contour values of density equal to 0.1 bohr^{-3} and 0.03 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 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.

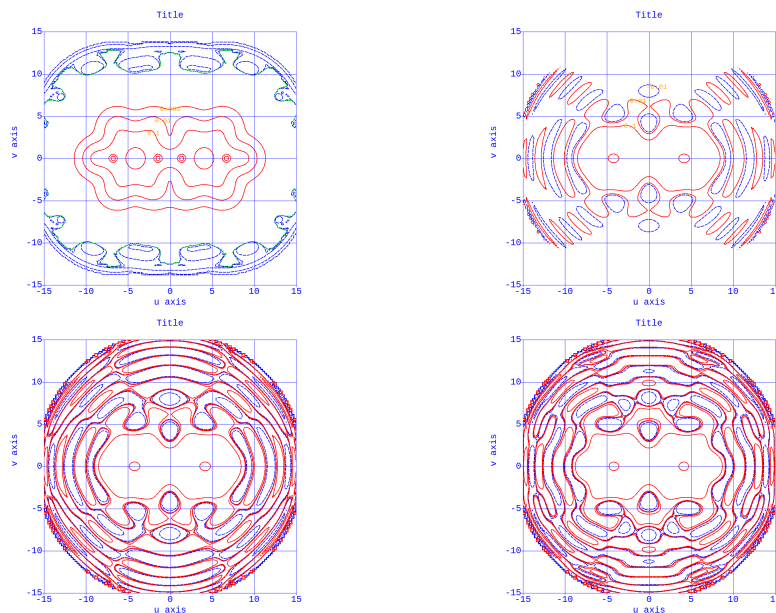


Figure 112: MED of biphenyl: upper-left: DAM expansion, remaining panels: Zernike-Canterakis expansions with different lengths

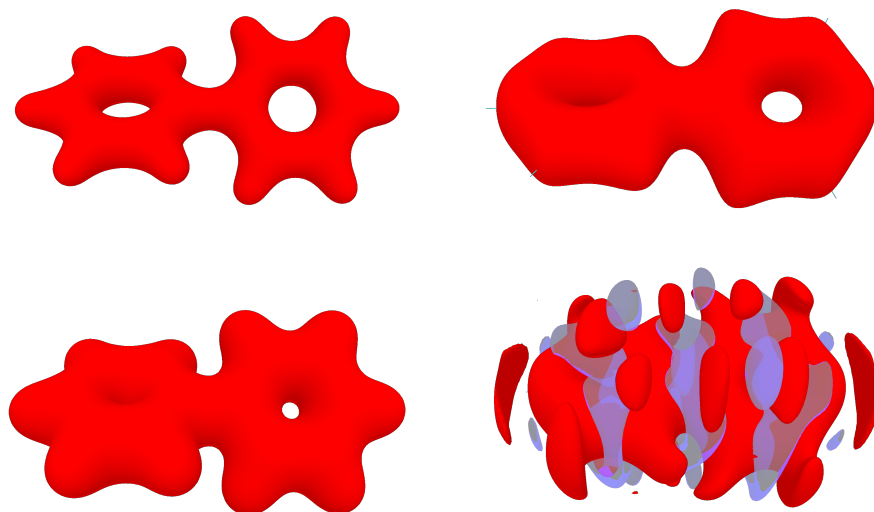


Figure 113: MED of biphenyl: left: DAM expansion, right: Zernike-Canterakis expansions; upper: contour 0.1 bohr^{-3} , lower: contour 0.03 bohr^{-3} (in blue: contour -0.03 bohr^{-3})

A Appendix: Format of files *.ggb*s and *.den*

The *.ggb*s 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 114):

Figure 114: *.ggb*s file structure

NCEN		Number of centers
X1 Y1 Z1 ZNUC1	}	Cartesian coordinates in bohr and nuclear charge of centers
X2 Y2 Z2 ZNUC2		
...		
NCONTR1		Number of contractions on first center
NPRIM11 L11	}	First contraction { No. of primitives; l quantum number primitive exponents contraction coefficients
EXP111 EXP112 EXP113 ...		
COEF111 COEF112 COEF113 ...		
NPRIM12 L12	}	Second contraction
EXP121 EXP122 ...		
COEF121 COEF122 ...		
...		
NCONTR2		Number of contractions on second center
NPRIM21 L21	}	First contraction
EXP211 EXP212 EXP213 ...		
COEF211 COEF212 COEF213 ...		
NPRIM22 L22	}	Second contraction
EXP221 EXP222 ...		
COEF221 COEF222 ...		
...		

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 ($ncontr_i$, integer) associated to the center followed, for each contracted function, by:

- one record with the number of primitives ($nprim_{i,j}$, integer) and the l quantum number associated to the contraction ($l_{i,j}$, integer)
- as many records as required with the primitive exponents ($exp_{i,j,k}$, real*8)
- as many records as required with the contraction coefficients ($coef_{i,j,k}$, 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, $T_k(t)$:

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

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 (ξ_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 requested 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 bohr².

Volume, \mathcal{V} : volume enclosed by the density isosurface in bohr³.

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

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

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 bohr².

Negative area, \mathcal{A}^- : area of density isosurface with negative MESP values, in bohr².

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

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

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

MESP variance, σ^2 : variance of MESP on isosurface in au² (Hartree²/ e^2).

Positive MESP variance, $(\sigma^+)^2$: variance of MESP on isosurface with positive MESP values in au² (Hartree²/ e^2).

Negative MESP variance, $(\sigma^-)^2$: variance of MESP on isosurface with negative MESP values in au² (Hartree²/ e^2).

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

ν 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, Ω , Ω^+ , Ω^- denote the corresponding total or partial isosurfaces.

$$\begin{aligned}\bar{V} &= \frac{1}{\mathcal{A}} \int_{\Omega} V(\mathbf{r}) dS & \bar{V}^+ &= \frac{1}{\mathcal{A}^+} \int_{\Omega^+} V(\mathbf{r}) dS & \bar{V}^- &= \frac{1}{\mathcal{A}^-} \int_{\Omega^-} V(\mathbf{r}) dS \\ (\sigma^+)^2 &= \frac{1}{\mathcal{A}^+} \int_{\Omega^+} [V(\mathbf{r}) - \bar{V}^+]^2 dS & (\sigma^-)^2 &= \frac{1}{\mathcal{A}^-} \int_{\Omega^-} [V(\mathbf{r}) - \bar{V}^-]^2 dS & \sigma^2 &= (\sigma^+)^2 + (\sigma^-)^2 \\ \Pi &= \frac{1}{\mathcal{A}} \int_{\Omega} |V(\mathbf{r}) - \bar{V}| dS\end{aligned}$$

F 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 udocked, values in spinboxes can be changed only with the right arrows. All the features are restored when the menu is docked back.

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