PRIMoRDiA 1.0v Tutorials

Igor Barden Grillo
(barden.igor@gmail.com)
github.com/igorChem

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Introduction

PRIMoRDiA (**PRI**MoRDiA **M**acromolecular **R**eactivity **D**escriptors **A**ccess) ia a shared memory parallel software written in C++ for post electronic structure calculations, that efficiently read output files from most used quantum mechanics packages, storing molecular information and processing it to generate several descriptors to evaluate the global and local reactivity of molecular systems. PRIMoRDiA supports the main reactivity descriptors of the Conceptual Density Functional Theory, the most famous and used reactivity theory, which work from response variables of the electronic structure of the molecules, as also other electrostatics properties.

Aknowlodgements

1 Tutorials

To learn how to use the program, its features and the auxiliary scripts, you can clone the repository from git hub with the following command

```
computer@user:$ git clone https://github.com/igorChem/PRIMoRDiA1.0v.git
```

Or paste this address in your web browser and download the zipped folder.

This repository contains output files for several quantum mechanical calculations needed to get the reactivity descriptors and input files examples for PRIMoRDiA. Also, this is the repository where you have access to the executable and this present document. In this section will be explore the results of PRIMoRDiA from these files.

1.1 Tutorial 1: Frozen Orbital Examples

1.2 Tutorial 2: Finite Differences Examples

1.3 Tutorial 3: Band Reactivity Descriptors Examples

1.4 Tutorial 4: Cube File Generation and Other Options

If you want generate total electron density or molecular orbitals cube files for the QM programs supported you can use the *"-ed"* or *"-mo"* flags respectively, as will be shown in the following examples. For small molecules, this files can be generated and visualized in common computational chemistry packages, such as Gabedit and Avogradro. Although, these software struggles very often for these tasks for molecules with more than one hundred atoms, then you can use PRIMoRDiA to generate the cube files.

The first example takes a Gaussian output for the acrolein molecule. In the folder where are the downloaded example files run the fol-

lowing command [1]to generate the total electron density grid with 40x40x40 of granularity

```
computer@user:$ primordia -ed acrloein_gauss.fchk 40 gaussian
```

The resulted file must have the *"acrloein_gauss.cube"* name. You can open it in pymol software invoking the command[2]

```
computer@user:$ pymol acrloein_gauss.cube
```
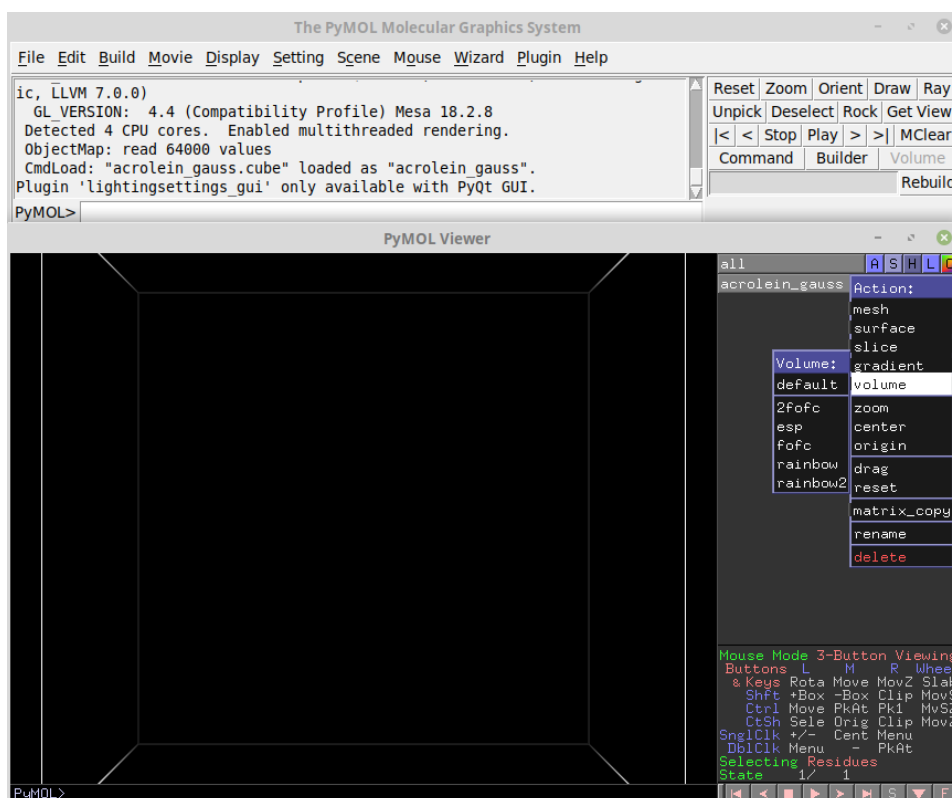

Figure 1: Pymol software window showing the right side bar with volume rendering options.

The Pymol window will open with the cube file loaded. To show the iso-surfaces go to the action options in the right side bar and click in *"volume"* and *"default"*, as showed in Figure 1. To save the image, write in the Pymol terminal emulator *"draw 800,600"* to render a 800X600 pixel images and *"png acrolein_gaus.png"* to save in png format, that is shown in Figure 2. This set of instructions

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[1] Tip: Put the PRIMoRDiA executable in .bashrc file with the following command: echo "alias primordia='/path/to/executable/PRIMoRDiA_1.0v'" » /home/user/.bashrc

[2] Tip: Install Pymol software from the linux command line. Try in command line: sudo apt install pymol

can be followed to generate the images from volume rendering in Pymol in the next tutorial steps.
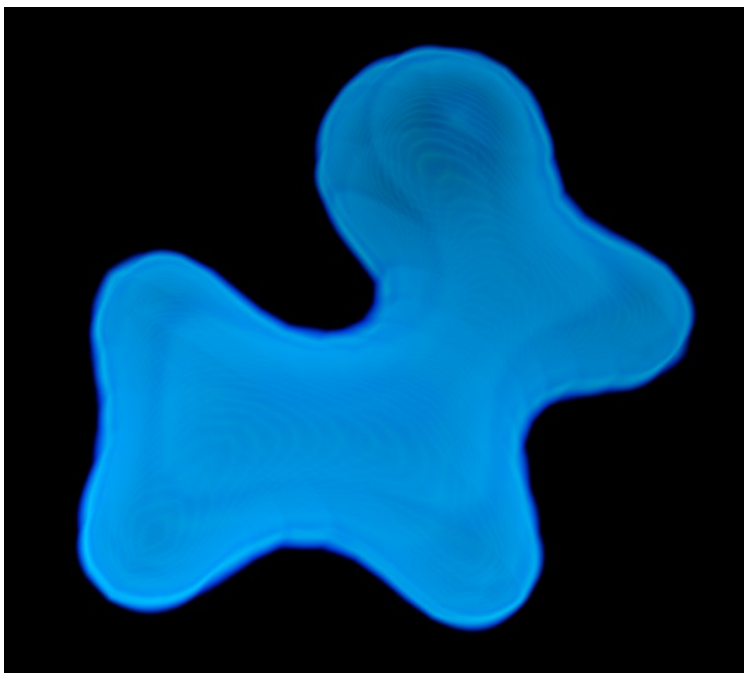

Figure 2: Acrolein total electron density calculated by PRIMoRDiA and saved from Pymol

The generation of Molecular Orbitals

```
computer@user:$ primordia -mo acrloein_gauss.fchk  40 gaussian
```

1.5 Tutorial 5: Chemical Reaction Analysis with PRIMoRDiA

1.6 Tutorial 6: Enzyme Reactivity

2 Dealing with Errors