GTKDynamo

Version 0.1.7

By

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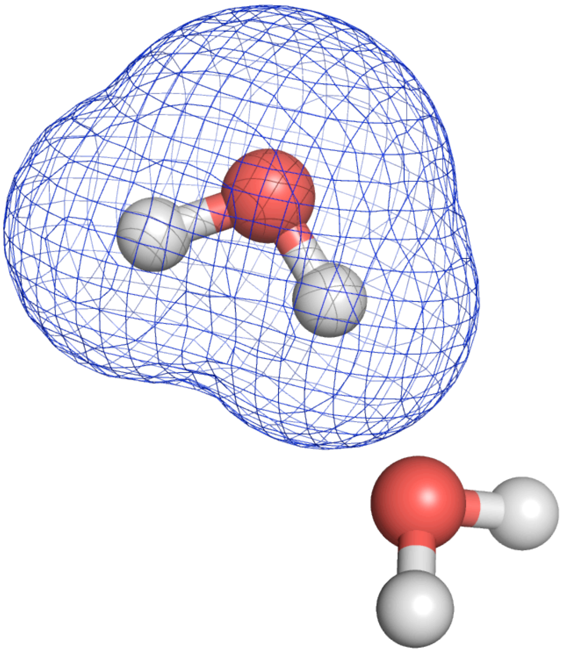
https://sites.google.com/site/gtkdynamo/



Summary

1. What is GTKDynamo?

GTKDynamo is free/open source software, which, together with pDynamo, transforms PyMol into a powerful interface for computational biochemistry and biophysics. The interface has been designed to facilitate the determination of reaction pathways in biological systems, specially using hybrid QC/MM (or QM/MM) methods. Pymol has been chosen as a graphical interface to pDynamo because it has a python API with wide documentation available.

1.1 Major features

GTKDynamo allows the users to perform most of kind of simulation method that pDynamo does, however with the facility of the graphic mode. The applications that GTKDynamo cover are:

- Pure QC simulations – *ab initio* and SMO
- Pure MM simulations – using AMBER, CHARMM or OPLS force fields
- Hybrid QC/MM simulations
- Single point calculations
- Energy minimization
- Molecular dynamics
- Reaction coordinate scanning
- Umbrella sampling
- Reactions path calculations
- and more…

2. Platforms

GTKDynamo is fully accepted on Linux (Ubuntu 12.04, OpenSuSe 12) and Mac OS X platforms. This interface was written in Python and make use of some external libraries that are essential to proper functioning, which are:

- pDynamo
- Matplotlib
- Numpy / Pylab
- PyMol 1.x
- pyGTK
- ORCA, *ab initio* calculations

3. Availability

GTKDynamo is free and the source files are available for Linux and Mac OS X.

4. License

5. Installation

5.1 Linux

5.1.1 External libraries

GTKDynamo required that some external libraries must be installed earlier. The linux repository can download four external libraries, if you are using Ubuntu just type:

- sudo apt-get install python-matplotlib python-numpy python-gtk* pymol

or if you are using OpenSuSe type:

- sudo zypper install python-matplotlib python-numpy-devel python-get-devel pymol

The pDynamo library installation is fully explained at the pDynamo website, the ORCA binary files can be downloaded at the website (http://www.mpibac.mpg.de/bac/logins/neese/description.php) and these binaries must been set in the PATH.

5.1.2 GTKDynamo

The GTKDynamo does not need to be installed, you just go the GTKDynamo folder and type:

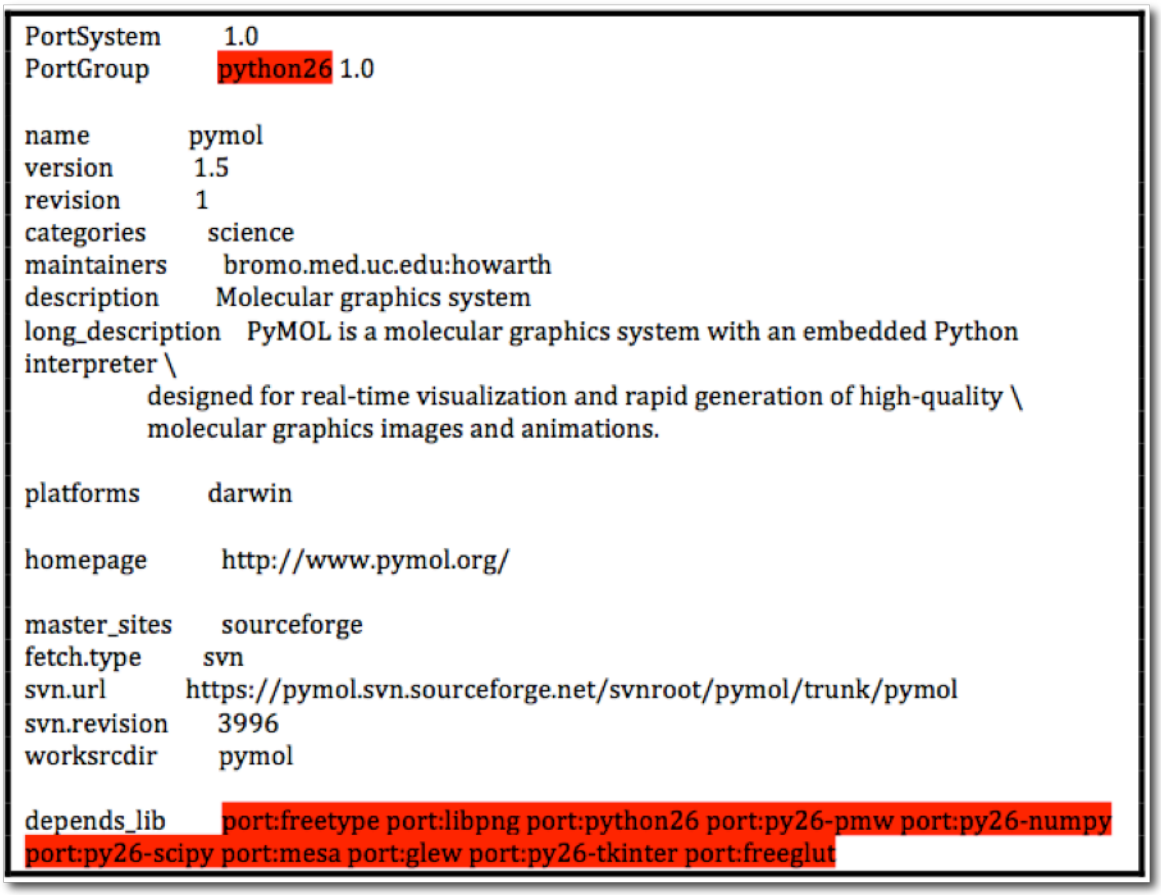
- pymol GTKDynamo.py

5.2 Mac OS X

The interface implementation on Mac OS X is fully accepted, however we just need to clarify some tricks about PyMol installation using MacPorts.
All Mac OS X users can download MacPorts (http://www.macports.org) to easily install programs, but sometimes we need to change some files to getthe right (or the more appropriate) libraries. We recommend using MacPorts to install PyMolp program with python 2.7. The default“Portfile” when we are using MacPorts to get PyMol is python 2.6, so we need to replace it by python 2.7 library.
Usually, MacPorts will create a new directory in your computer (/opt/local). All programs will be installed using the information provided by the “Portfile”, and it's this file thatwe have to edit. Do itis simple.Go to the terminal and type:

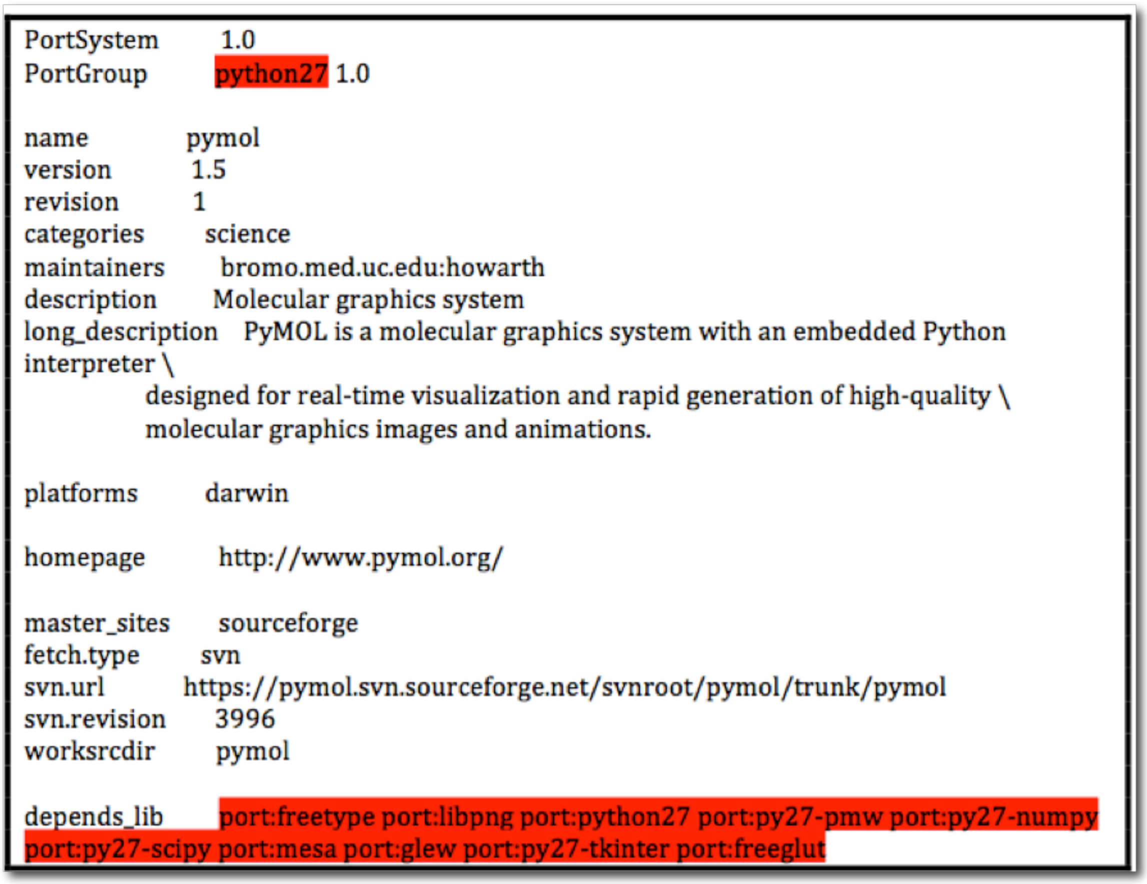
```
$ cd opt/local/var/macports/sources/rsync.macports.org/release/tarballs/ports/science/pymol/
```

In this folderwe have to editthe “Portfile”file:



```
PortSystem       1.0
PortGroup        python26 1.0

name             pymol
version          1.5
revision         1
categories       science
maintainers      bromo.med.uc.edu:howarth
description      Molecular graphics system
long_description    PyMOL is a molecular graphics system with an embedded Python
interpreter \
                 designed for real-time visualization and rapid generation of high-quality \
                 molecular graphics images and animations.

platforms        darwin

homepage         http://www.pymol.org/

master_sites     sourceforge
fetch.type       svn
svn.url          https://pymol.svn.sourceforge.net/svnroot/pymol/trunk/pymol
svn.revision     3996
worksrcdir       pymol

depends_lib      port:freetype port:libpng port:python26 port:py26-pmw port:py26-numpy
port:py26-scipy port:mesa port:glew port:py26-tkinter port:freeglut
```

In this file we have to change the parts highlighted in red to:



```
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name            pymol
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platforms       darwin

homepage        http://www.pymol.org/

master_sites    sourceforge
fetch.type      svn
svn.url         https://pymol.svn.sourceforge.net/svnroot/pymol/trunk/pymol
svn.revision    3996
worksrcdir      pymol

depends_lib     port:freetype port:libpng port:python27 port:py27-pmw port:py27-numpy
port:py27-scipy port:mesa port:glew port:py27-tkinter port:freeglut
```

After, just type:

```
$ sudo port install pymol
```

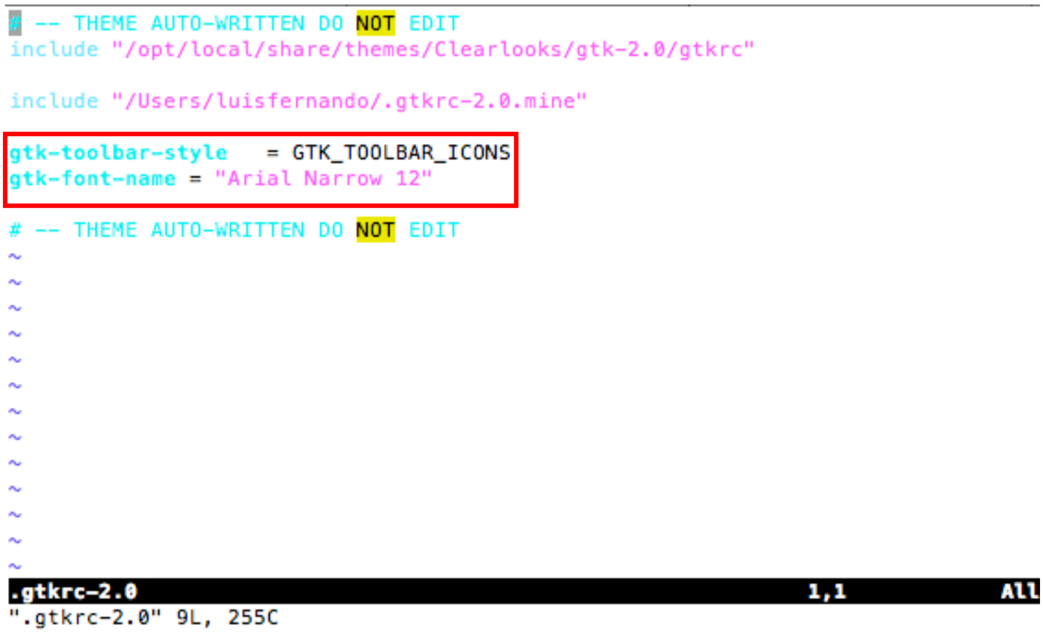
This command will install PyMol with python 2.7. Since GTK_Dynamo requires GTK and Matplotlib libraries, type:

```
$ sudo port install py27—gtk py27—matplotlib
```

After these libraries were installed, your GTK_Dynamo interface should work properly. However, we need to perform one more step to setup GTK Dynamo in a fashionable way, to type:

```
$ vi .gtkrc-2.0
```

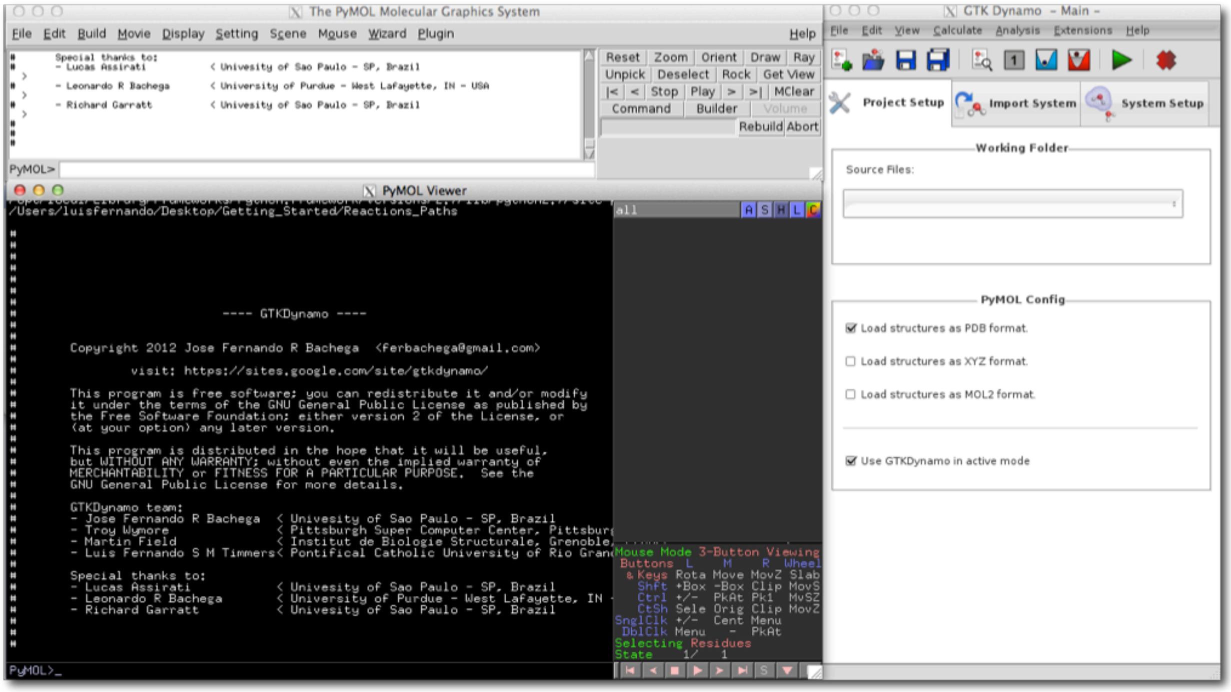
and add this highlighted lines:



```
# -- THEME AUTO-WRITTEN DO NOT EDIT
include "/opt/local/share/themes/Clearlooks/gtk-2.0/gtkrc"

include "/Users/luisfernando/.gtkrc-2.0.mine"

gtk-toolbar-style    = GTK_TOOLBAR_ICONS
gtk-font-name = "Arial Narrow 12"

# -- THEME AUTO-WRITTEN DO NOT EDIT
~
~
~
~
~
~
~
~
~
~
~
~
~
~
.gtkrc-2.0                                              1,1           All
".gtkrc-2.0" 9L, 255C
```

To check if the interface works well, go to GTK_Dynamo folder and type:

$ pymol GTK_Dynamo.py



The PyMOL Molecular Graphics System
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help
Reset Zoom Orient Draw Ray
Unpick Deselect Rock Get View
|< < Stop Play > >| MClear
Command Builder Volume
Rebuild Abort
PyMOL Viewer
all
A S H L C
GTK Dynamo - Main -
File Edit View Calculate Analysis Extensions Help
Project Setup
Import System
System Setup
Working Folder
Source Files:
PyMOL Config

```
#       Special thanks to:
#       - Lucas Assirati          < Univesity of Sao Paulo - SP, Brazil
 >
#       - Leonardo R Bachega      < University of Purdue - West Lafayette, IN - USA
 >
#       - Richard Garratt         < Univesity of Sao Paulo - SP, Brazil
 >
#
#
#
PyMOL>
```

```
/Users/luisfernando/Desktop/Getting_Started/Reactions_Paths

#
#
#
#
#
#
#
#                      ---- GTKDynamo ----
#
#
#      Copyright 2012 Jose Fernando R Bachega  <ferbachega@gmail.com>
#
#              visit: https://sites.google.com/site/gtkdynamo/
#
#      This program is free software; you can redistribute it and/or modify
#      it under the terms of the GNU General Public License as published by
#      the Free Software Foundation; either version 2 of the License, or
#      (at your option) any later version.
#
#      This program is distributed in the hope that it will be useful,
#      but WITHOUT ANY WARRANTY; without even the implied warranty of
#      MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.  See the
#      GNU General Public License for more details.
#
#      GTKDynamo team:
#      - Jose Fernando R Bachega  < Univesity of Sao Paulo - SP, Brazil
#      - Troy Wymore              < Pittsburgh Super Computer Center, Pittsbur
#      - Martin Field             < Institut de Biologie Structurale, Grenoble,
#      - Luis Fernando S M Timmers< Pontifical Catholic University of Rio Gran
#
#      Special thanks to:
#      - Lucas Assirati           < Univesity of Sao Paulo - SP, Brazil
#      - Leonardo R Bachega       < University of Purdue - West Lafayette, IN -
#      - Richard Garratt          < Univesity of Sao Paulo - SP, Brazil
#
#
#
PyMOL>_
```

```
Mouse Mode 3-Button Viewing
Buttons  L    M    R  Wheel
 & Keys Rota Move MovZ Slab
   Shft +Box -Box Clip MovS
   Ctrl +/-  PkAt Pk1  MvSZ
   CtSh Sele Orig Clip MovZ
SnglClk +/-  Cent Menu
 DblClk Menu  -   PkAt
Selecting Residues
State    1/   1
```

☑ Load structures as PDB format.

☐ Load structures as XYZ format.

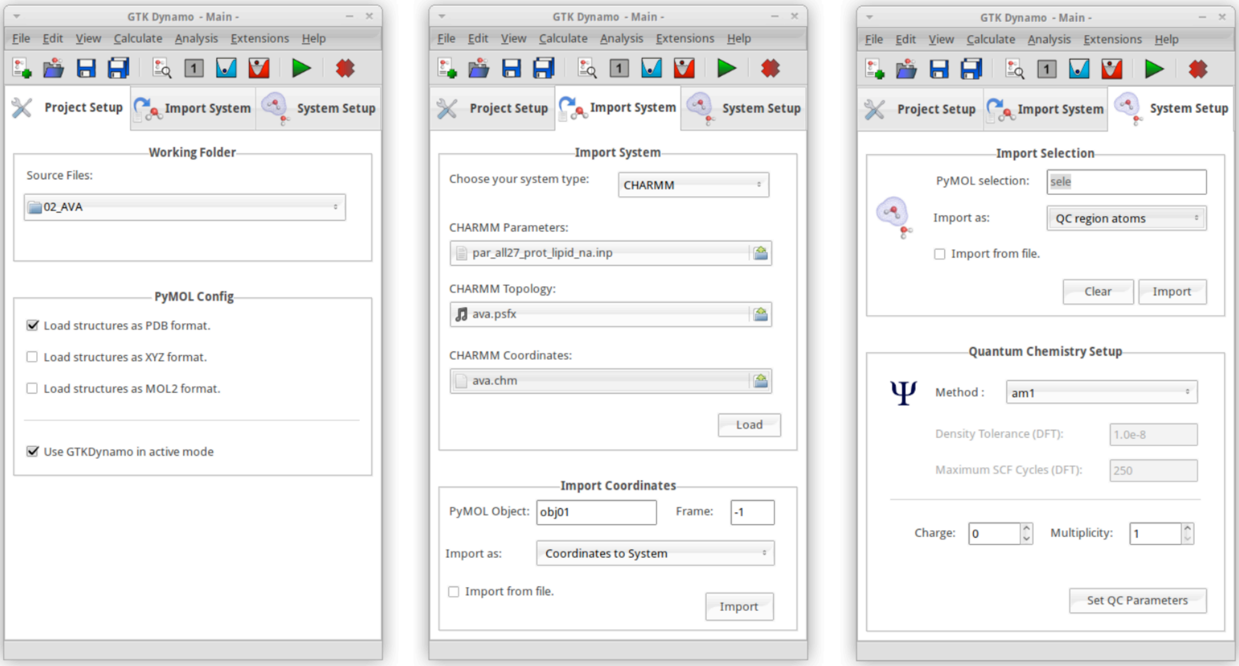
☐ Load structures as MOL2 format.

☑ Use GTKDynamo in active mode

6.Operating GTKDynamo

6.1 Basic about GTKDynamo interface

GTKDynamo interface should be understood as a pDynamo extension, where the objective is; (1) provide a graphical interface able to handle the data generated by pDynamo, and (2) cover the most of the main capabilities available in pDynamo. GTKDynamo main window can be split out into three parts: Main menu, Toolbar and Notebook (figure 1).



Source Files: 02_AVA

☑ Load structures as PDB format.
☐ Load structures as XYZ format.
☐ Load structures as MOL2 format.
☑ Use GTKDynamo in active mode

Choose your system type: CHARMM
CHARMM Parameters: par_all27_prot_lipid_na.inp
CHARMM Topology: ava.psfx
CHARMM Coordinates: ava.chm

PyMOL Object: obj01 Frame: -1
Import as: Coordinates to System
☐ Import from file.

PyMOL selection: sele
Import as: QC region atoms
☐ Import from file.

Method : am1
Density Tolerance (DFT): 1.0e-8
Maximum SCF Cycles (DFT): 250
Charge: 0 Multiplicity: 1

Figure 1: *GTKDynamo overview.*

6.2 Menus

Program functions may be accessed using pull-down menus under the items in the main menu bar (figure 1), for example, the “*File*” menu.

- **File**

  Allows the user to create a new project (see section *Getting started*) or read one of it that has previously saved. The user can also load pkl files (the pDynamo serialization files), coordinates and trajectories.

- **Edit**

  Allows the user handle selections using pDynamo selections tools, rescale charges, merge objects (PyMOL) and setup system parameters, such as non-bonded interactions parameters.

- **View**

  Allows the user call for the auxiliary windows available in GTKDynamo. This option is similar to the trajectory handler window.

- **Calculate**

  This menu item includes many tools that cover most of the capabilities of pDynamo. Here the user will be able to call for process like: single point calculations, energy minimization, molecular dynamics, normal modes calculations, surface calculations (e.g. electron density in QC or QC/MM systems), and many tools specially designed to perform reaction path calculations.

- **Extensions**

  This Item menu contains tools designed to interface GTKDynamo with external programs, such as Ambertools and GROMACS.

- **Help**

  Here the user will find a link to the tutorials and the credits about the GTKDynamo.

6.3 Toolbar items

The toolbar is a faster and optimized way to access the most frequently used functions available in GTKDynamo. The actual version has ten toolbar buttons:

- **New project**

  This button summarizes the first two tabs and presents some additional options. The “*Working folder*” can be choose here and is allowed to the user set a “*Project name*” and if is desirable to do “*Backup source files*”. Similar to “*Import System*” tab, the system can be load as one of the three force fields available at the moment (AMBER, CHARMM or OPLS) or with a pkl file. Furthermore, other options such as “*Non-bonded Models*”, “*Periodic bound conditions*” and “*pDynamo/PyMol Config*” can be selected.

- **Open GTKdynamo project**

  Allows the users load GTKDynamo projects in three different extensions file (GTKDyn, PKL and YAML).

- **Save**

  This button is a easy way to keep your system saved, since you have been already saved.

- **Save as project**

  When the user click on this option, the project will be saved in three different formats (GTKDyn, PKL and PSE) with the respective name furnished by the user.

- **Check System**

  Print the system parameters in the terminal.

- **Single point**

  This button performs a single point calculation of the active system.

- **Energy minimization**

  Here the users can execute energy minimizations process with two different algorithms (Conjugated Gradient and Steepest Descent).

- **Molecular Dynamics**

  Similar to “Energy Minimization” button, here the users have the possibility to perform a molecular dynamics simulation with one of the three velocity integrators available in the pDynamo library (Velocity Verlet Dynamics, Leap-frog Dynamics or Langevin Dynamics).

- **Trajectory visualization tool**

  Allows the users monitor the trajectory frames after it is loaded.

- **Delete system**

  Allows the users clear all system parameters.

6.4 Tabs

Finally, the notebook contain the three tabs that was created to provide to the user the most important tools to setup the project variables, interchange coordinates and edit system.

- **Project Setup**

  Here the user will be able to setup where the files (some of them temporary) will be generated. Allows the user setup what kind files GTKDynamo will interchange with PyMOL (PDB is strongly recommended) and how GTKDynamo will be connected with PyMOL (Active/Passive mode). If the option “Use GTKdynamo in active mode” is active, the interface will check for any possible structural modification in the last PyMOL object generated by GTKDynamo, providing to the user a higher interactive experience in molecular modeling using GTKDynamo.

- **Import System**

  This tab contains all the tools to load in memory an external system supported by pDynamo. Four options are available at the moment:

  - **AMBER**
  - **CHARMM**
  - **GROMACS**
  - **OPLS** – generated in pDynamo

  There is also a special box to import coordinates from files, or from any PyMOL object. This is a very useful tool, once that any PyMOL object can be easily loaded in memory, turn the PyMOL session also a backup from the passed steps.

- **System Setup**

  This tab has been designed to handle with the selections previously generated in PyMOL. Three types of operations can the done:

  - Fix atoms – the imported atom list will be fixed
  - Prune atoms – used to reduce the system, all the atoms not included in the selection will be removed
  - QC region atoms – put the selected atoms in a QC region – used in Hybrid

simulations.

The quantum chemistry box allows the user choose for one of all the QC theory levels available in pDynamo. If the option “ORCA ab initio” has been choose, a new window will rise where a more specific customization should be done. After the choice, the user should chick on button “Set QC Parameters”, if a selection has previously imported as “QC region atoms”, a Hybrid system will be generated, in the other hand, all the atoms will be include in the QC region.

6.5 The GTKDynamo format

When a GTKDynamo project is created, three related files are generated:

- **a pkl file** (pDynamo serialization file),which contains all the information about the system (fixed atoms, QC atoms, parameters, coordinates etc...). This file itself is compatible with GTKDynamo and can be load in memory or transferred to and desired place.
- **a pse file** (pymol serialization file), which contains all the information from the PyMOL session (object, selections, configurations etc...)
- **a gtkdyn file** (GTKDynamo project file), which is a very simple text file connecting the pkl and the pse file, and also information about what was the last step executed by user and from which PyMOL object GTKDynamo is connected.

So, when should I use pkl files and when should I use GTKDynamo projects ?

The pkl files are portable and can be transferred from one place to another. They are fully interpreted by GTKDynamo, and can be used as starting point to a more specific simulation using a custom scripts. A GTKDynamo project should be created when all the information at the PyMOL session are relevant and should be keep.

When create a new project in GTKDynamo, a pkl file is also generated. Is it the same file as any other pkl from pDynamo?

Yes.

So, could be loaded in memory by itself?

Yes.