

OpenDx Tools for InteGriTy

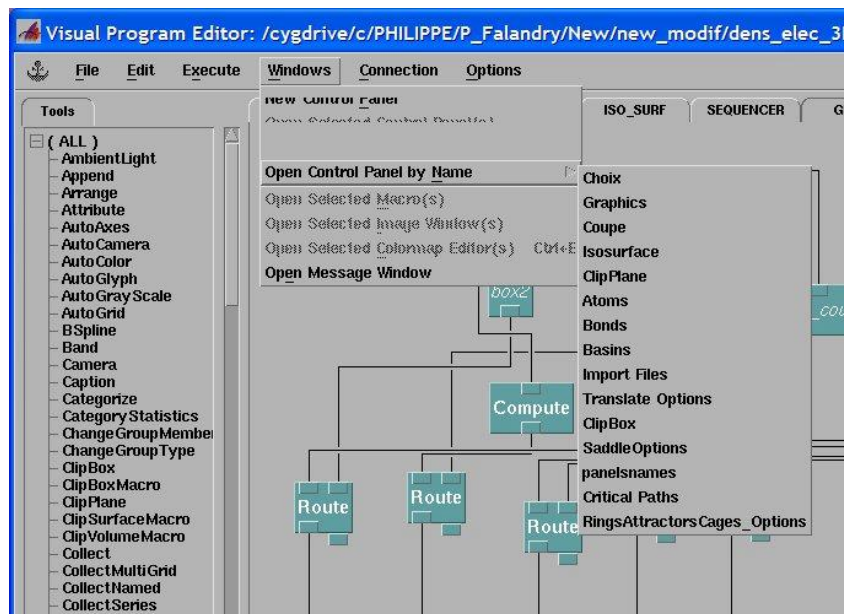
Get Started

Once you have installed OpenDx, launch it in the edit mode and give the location of the complementary macros (macros_directory and prog_directory can be the same).

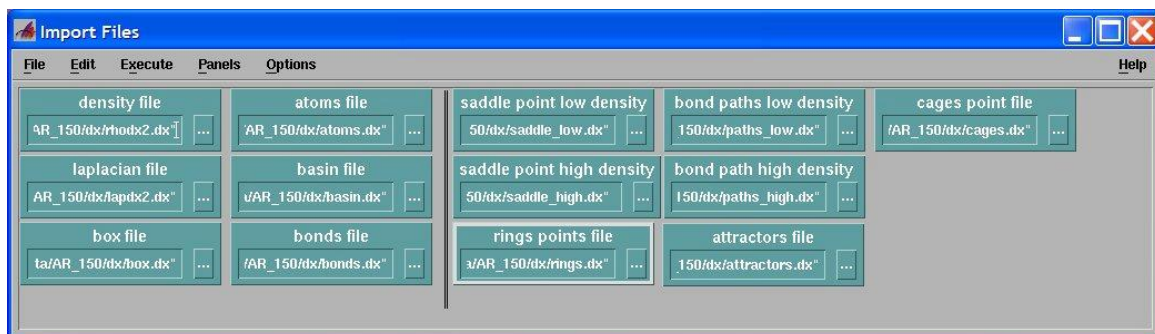
```
$ dx -macros /macros_directory -edit -memory 800 /prog_directory/dens_elec_3D_813.net ←
```

The “Visual Program Editor” should appear.

Select in the menu-bar “Windows/Open Control Panel by Name/Import Files” to give correct pathways and data filenames

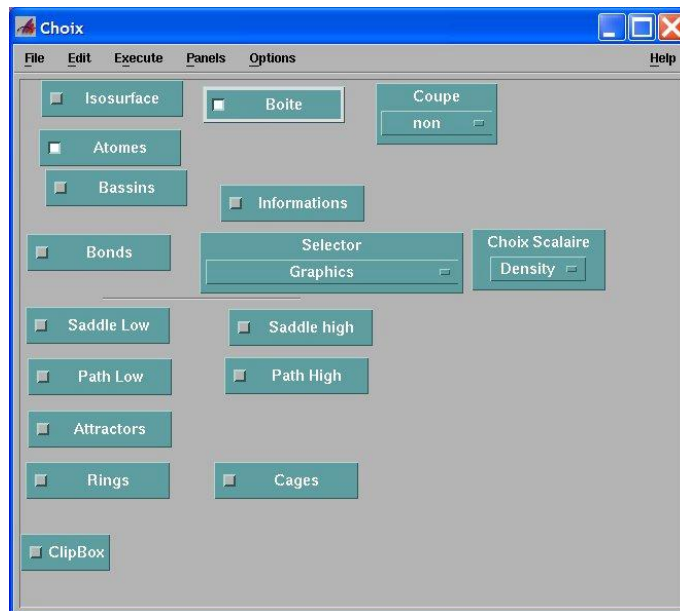


This would look like the following:



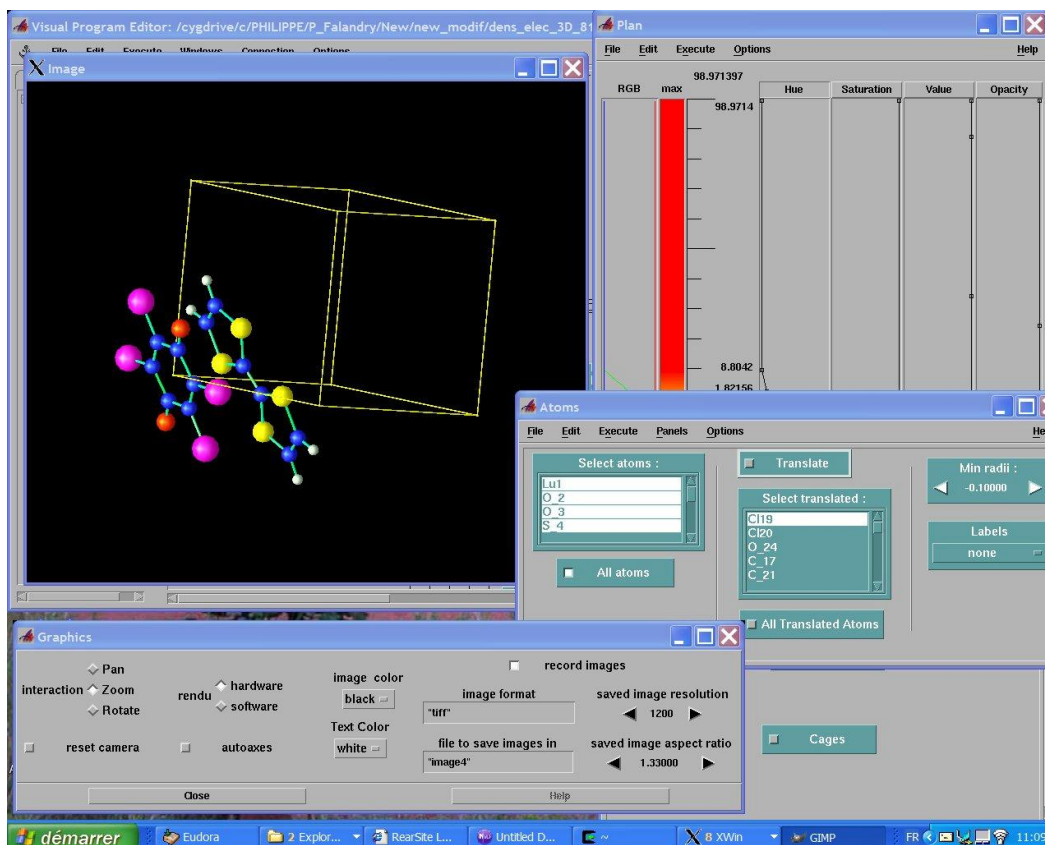
Then for each kind of data to be plotted (density, laplacian, atoms, bonds, basins, critical points and bondpaths) select the corresponding file that have been produced by InteGriTy or CpGriTy output routines. When running InteGriTy or CpGriTy you have first to create a subdirectory named “dx”

Select menu “**Windows/Open Control Panel by Name/Choix**” to select operations to be executed



Then select “**Execute**” in any window’s menu-bar. Some actions may not run correctly in the “execute on change” mode (too slow...).

The “**Image**” window and auxiliary windows should appear, just like given below as example.



Then just play with all control panels and find out what are all the possibilities and bugs ... which you could find and report all of them ...