Compiling the Debussy Suite on UNIX systems with Anaconda

Preliminary requirements

1) You MUST have **Anaconda Python** installed. If not, download the **Anaconda3 Python 3.9 version** from

https://www.anaconda.com/products/individual

After launching the installer, please pay attention at the following options:

Destination Select: Select Machintosh HD=> click on Choose Folder button and select /Users/*your_username* as installation folder (check the message related to the chosen folder)

Installation type=> click on "ad hoc" button => disable modify PATH (under package name: Anaconda3)=> click Install

VERY IMPORTANT: the installation requires at least 5GB free for storage.

If you have already another python3.X version installed on your pc, please check the presence of matplotlib, numpy and wxpython libraries. If not there, please install them with pip3:

(python3 path)pip3 install wxpython

And the same for the other missing libraries.

For Linux system only: if the installation of wxpython gives errors, please try first installing **python3–wxgtk4** (or other versions, depending on the OS) from the OS repositories. For example, for Linux-gnu systems it will be:

sudo apt-get install python3– wxgtk4

2) You MUST have **gfortran** and **gcc** compilers (suggested version <= 6.0) installed. You can download them from *homebrew* repositories (https://brew.sh both for Linux and MacOSX systems).
The compilers must be properly linked and called by the system directly as **gcc** and **gfortran**, as required by the makefile of the suite.

3) **For MacOSX systems only:** you must install XQuartz. It can be downloaded the dmg from the following website: www.xquartz.org and installed.

IMPORTANT: Restart your computer after installing XQuartz!

4) **For Linux systems only:** be sure to have xterm installed (e.g. by **sudo apt-get install xterm** ..)

3) You MUST have **Java** installed for running **Jmol-13.0.08** package, which is used as the visualization tool of atomistic models in Debussy. **Jmol-13.0.08** is provided with the Suite. However, **Java** is required. Download and install it from **www.java.com** (it is suggested to download the last version available on the website: Java version older than April 2019 may give some issues, due to modification in the Oracle Java license).

4) We suggest having the package **Mercury** (available for free from the Cambridge Crystallographic Data Center – CCDC) as an integrative visualization tool, downloadable from. www.ccdc.cam.ac.uk/Solutions/FreeSoftware/pages/FreeMercury.aspx

Debussy Suite installation

1) Download from https://github.com/DeByeUSerSYstem/DEBUSSY_v2.2-UNIX the Suite by clicking on the green button Code ➔ **Download ZIP** and unzip DEBUSSY_v2.2-UNIX -main.zip.

2) Unzip the file and move the DEBUSSY_v2.2 subfolder from the subfolder UNIX to **/Users/*your_username*** (or **/home/*your_username*** depending on your system)
Some executables must need permissions to be executed under your *User* account.
To do so, please type on a Terminal:

chmod +x /Users/*your_username*/DEBUSSY_v2.2/install_debussy_v2.2
chmod -R +x /Users/*your_username*/DEBUSSY_v2.2/extlib

3) In order to compile the Debussy- Suite, using a terminal, move into the folder DEBUSSY_v2.2, by typing:

cd /Users/*your_username*/DEBUSSY_v2.2

You are ready to install the Debussy Suite. You need root credentials for this operation. Type on the command line:

./install_debussy_v2.2

You will be asked three important questions:

a) insert the installation folder. Use the full path:

/Users/*your_username*/DEBUSSY_v2.2

b) compiling the external lib (LAPACK, LCREF, NLOPT), type YES (**Y**)

c) installing the Graphical User Interface (GUI), type YES (**Y**)

d) [if you are working on a linux-gnu platform (Ubuntu or Debian)] downloading lapack and blas from system repositories, type YES (**Y**)

The installation can take some min. At the end of the procedure, you will have a message "DONE!!' and "BYE BYE" on your terminal window.

Check that 16 binaries have been created in the **DEBUSSY_v2.2/bin** subfolder.

4) Inside the **DEBUSSY_v2.2** folder you can find a **RUN_TEST_UNIX** folder, containing some files to test the Debussy workflow. Type on the Terminal:

cd RUN_TEST_UNIX
sh drun

The output of the program should appear on the Terminal ending with "******* Debussy simulation DONE! *******".
The installation of the Debussy Suite is successfully completed.

5) Check the GUI installation, by typing on the command line (in the **DEBUSSY_v2.2/bin** folder):

./debussy-suite_gui

If you see on your screen the GUI as in the image below, the GUI installation procedure ended successfully. Otherwise, you will have error messages on the terminal window, please send them to us (Federica.bertolotti@uninsubria.it; Antonella.guagliardi@ic.cnr.it), we will try to help you in solving the problems.

Data for Tutorials

Download the archive **TUTORIALS-main.zip** from https://github.com/DeByeUSerSYstem/TUTORIALS, by clicking on Code -> Download ZIP
Unzip it and save it in any location under your User.
VERY IMPORTANT: Please DON'T USE BLANK SPACES in the full path of the folder.

the Debussy Team