Installing the Debussy Suite on Mac OSX 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.

2) 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!

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) Move the DEBUSSY_v2.2 folder from the subfolder macOSX to **/Users/*your_username***

3) Launch a Teminal from Applications => Utilities.

4) Move into the folder **DEBUSSY_v2.2** to install the programs Suite, by typing on a Terminal:

cd /Users/*your_username*/DEBUSSY_v2.2

You are ready to install the Debussy Suite. Type on the Terminal:

./install_debussy_v2.2

At some point you will be asked for root credentials (to be inserted).
This will allow to move some library provided by us, in the /usr/local/* and /opt/local/* folders. During this step the anaconda3 and DEBUSSY_v2.2 paths will be added at the User environmental variable. Also, a missing python library (wxpython) will be installed.
The installation can take some minutes. At the end of the procedure, you will have a message "DONE!!' and "BYE BYE" on your terminal window.

5) 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.
The following instructions are required for installing the GUI.

6) Check the GUI installation, by double clicking on the **debussy-suite_gui** launcher in **DEBUSSY_v2.2** folder.

If you can see on your screen the GUI appearing, the installation procedure ended successfully.
Otherwise, to understand the error, **drag and drop the debussy-suite_gui launcher on the Terminal** (a new one with respect to the previous installation) and press enter. You will read error messages on the Terminal window and send it to us.

If the GUI installation ended successfully, you can drag & drop the debussy-suite_gui launcher in your dock or on your desktop.

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