Installing the Debussy Suite on Mac OSX systems with Anaconda Python 3.9

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 the installation 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 from the following website: www.xquartz.org and then 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 the Suite from https://github.com/DeByeUSerSYstem/DEBUSSY_v2.2-UNIX by clicking on the green button **Code** ➔ "Download ZIP" and unzip *DEBUSSY_v2.2-UNIX -main.zip*.

2) Enter in the *macOSX* subfolder and move the DEBUSSY_v2.2 subfolder to **/Users/*your_username***

3) Launch the Teminal (from Applications => Utilities).

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

cd /Users/*your_username*/DEBUSSY_v2.2

You are ready to install the Debussy Suite.

Type on the Terminal command line:

./install_debussy_v2.2

You will be asked for root credentials (to be inserted).
This will allow some libraries provided by us to be moved in the /usr/local/* and /opt/local/* folders. During this step the Anaconda3 and DEBUSSY_v2.2 paths will be added to 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 command line:

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.

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 a new Terminal and press enter. You will read error messages on the Terminal window; copy and send them to us.

If the GUI installation ended successfully, you can drag & drop the debussy-suite_gui launcher on 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