Compiling the Debussy Suite on UNIX systems with Anaconda Anaconda Python3

Preliminary requirements

1) You MUST have **Anaconda Python** installed. If not, then download the latest version of Anaconda3 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.

- Wxpython is missing from the Anaconda package (and it is needed for running the Debussy GUI). Please install it, by typing on a terminal:

  pip3 install wxpython

  (NB. Don't use *conda install* ***!)

- **For Linux system only:** if the installation of wxpython gives errors, please try first installing **python3– wxgtk4.0** (or newer versions, depending on the OS) from the OS repositories:

  sudo apt-get install python3– wxgtk4.0

- If you have another Python3 version already installed on your PC (or do you prefer to save disk space, by installing Python3 from scratch: https://www.python.org/downloads/), please install the required libraries (matplotlib, numpy, wxpython), by typing on a terminal:

  (*Python3 path*)pip3 install *library*

2) You MUST have **gfortran** and **gcc** compilers 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
(e.g. ln -s /usr/bin/gcc-13 /usr/bin/gcc
ln -s /usr/bin/gfortran-13 /usr/bin/gfortran)

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 -R 777 /Users/*your_username*/DEBUSSY_v2.2

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.