

# 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 (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](http://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](http://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](http://www.ccdc.cam.ac.uk/Solutions/FreeSoftware/pages/FreeMercury.aspx)

## Debussy Suite installation

1) Download from [https://github.com/DeByeUserSYstem/DEBUSSY\\_v2.2-UNIX](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, LCREP, 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.