Installing the Debussy Suite on 64-bit Windows systems with Anaconda

Preliminary requirements

1) Python 3.9 is not compatible with Windows <=7. If you don't have at least Windows 8 installed on your pc, please contact us for suggestions on alternative Python3 versions.

2) You MUST have **Anaconda3 Python** installed:
   If you do not have any previous Python version already installed, then download the **Anaconda3 Python 3.9 version** from

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

VERY IMPORTANT:

- installation requires at least 5.70GB free for storage.
- During installation is strongly suggested to select the installation "Just me (recommended)" (=under the current User), and the option "Add Anaconda3 to my PATH environmental variable", although not recommended by the installer.

if you have a previous Python version installed, please contact us at
Federica.bertolotti@uninsubria.it; Antonella.guagliardi@ic.cnr.it

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 modifications in the Oracle Java license).

4) Recommended**:** 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-WINDOWS the Suite by clicking on the green button Code ➜ Download ZIP and unzip DEBUSSY_v2.2-WINDOWS-main.zip.

Enter in the WINDOWS folder and move the cygwin64 folder from the WINDOWS subfolder to C:\
Any other location is not handled

You have now **a C:\cygwin64** folder containing three parallel subfolders:

C:\cygwin64\bin (containing the windows .dll)
C:\cygwin64\DEBUSSY_v2.2 (containing the DebUsSy Suite binaries, GUI and launcher)
C:\cygwin64\RUN_TEST_WIN (Test Run for Debussy, to run after the installation)

and a batch file (i.e. a Windows script):
C:\cygwin64\ DEBUSSY_v2.2\install_v2.2.bat (Debussy installer)

5) Double click on the **install_v2.2.bat** file (click on the option "Run as administrator" with the right mouse button): this batch file will update the System variable Path, by adding the C:\cygwin64\bin path and it will install the wxpython module that is missing in the Anaconda3 package.

- If the automatic setting of the environmental variables fails, update the User or (if possible) System variable Path by yourself (by adding C:\cygwin64\bin\, as explained here: https://www.opentechguides.com/how-to/article/windows-10/113/windows-10-set-path.html).
  If the automatic wxpython installation fails, type from Anaconda prompt (look for it in the Windows Search Menu):

pip install -U wxpython

3) **Double click** on the **debussy-suite_GUI.bat** *shortcut* (under C:\cygwin64\DEBUSSY_v2.2\) for launching the GUI of the Suite. (you can also create a desktop shortcut and associate the debussy-icon.ico available in the folder).
If you see on your screen the GUI opening, the GUI installation procedure ended successfully.
Otherwise, to understand the error, we suggest to do the following operations: under **C:\cygwin64\DEBUSSY_v2.2\bin** you will find the **debussy-suite_GUI.bat** *batch file.* Drag and drop it on the Windows command prompt and press enter.
You will read an error message on the terminal window and send it to us if you need support (Federica.bertolotti@uninsubria.it; Antonella.guagliardi@ic.cnr.it).

If you want to create a desktop shortcut, you can link the icon *debussy-icon.ico* available in the **C:\cygwin64\DEBUSSY_v2.2** folder to the **debussy-suite_GUI.bat** *shortcut* and copy it on your desktop.

4) Open the **C:\cygwin64\RUN_TEST_WIN** and double click on **drun.bat**.
The run-time output of the program should appear on the Terminal ending with "Debussy simulation done". If not you will read an error message and send it to us if you need support (Federica.bertolotti@uninsubria.it; Antonella.guagliardi@ic.cnr.it).

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