

Installing the Debussy Suite on 64-bit Windows systems with Anaconda Python3 (for the Debussy GUI)

Preliminary requirements

- 1) You MUST have **Anaconda3 Python** installed:
If you do not have any previous Python version already installed, then download the latest version of **Anaconda3** 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 both 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 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 and wxpython):

(Python3 path)pip install library

- 2) 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).
- 3) 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* subfolder and move the *cygwin64* subfolder to C:\

Any other location is not handled

You have now the **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)
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2) Double click on the **install_v2.2.bat** file (click on the option as “Run as administrator” using the right mouse button): this batch file updates the System variable Path (by adding the C:\cygwin64\bin path) and installs the wxpython module (missing in Anaconda3 package).

- If the automatic setting of the environmental variables fails (if your User has not Administrator privileges), you have to update the *User* or (if possible) *System* variable Path by yourself (by adding C:\cygwin64\bin\). If necessary, follow the guidelines here: <https://www.opentechguides.com/how-to/article/windows-10/113/windows-10-set-path.html>.
- If the automatic wxpython installation fails, type from the Anaconda prompt (look for it in the Windows Search Menu):

pip install wxpython

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

3) Double click on the **debussy-suite_GUI.bat** *shortcut* (under **C:\cygwin64\DEBUSSY_v2.2**) for launching the GUI of the Suite.

If you see on your screen the GUI opening, the installation procedure ended successfully.

Otherwise, to understand the error, we suggest doing the following operations: in **C:\cygwin64\DEBUSSY_v2.2\GUI** 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; 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 to 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; copy it, and send it to us (Federica.bertolotti@uninsubria.it; Antonella.guagliardi@ic.cnr.it).