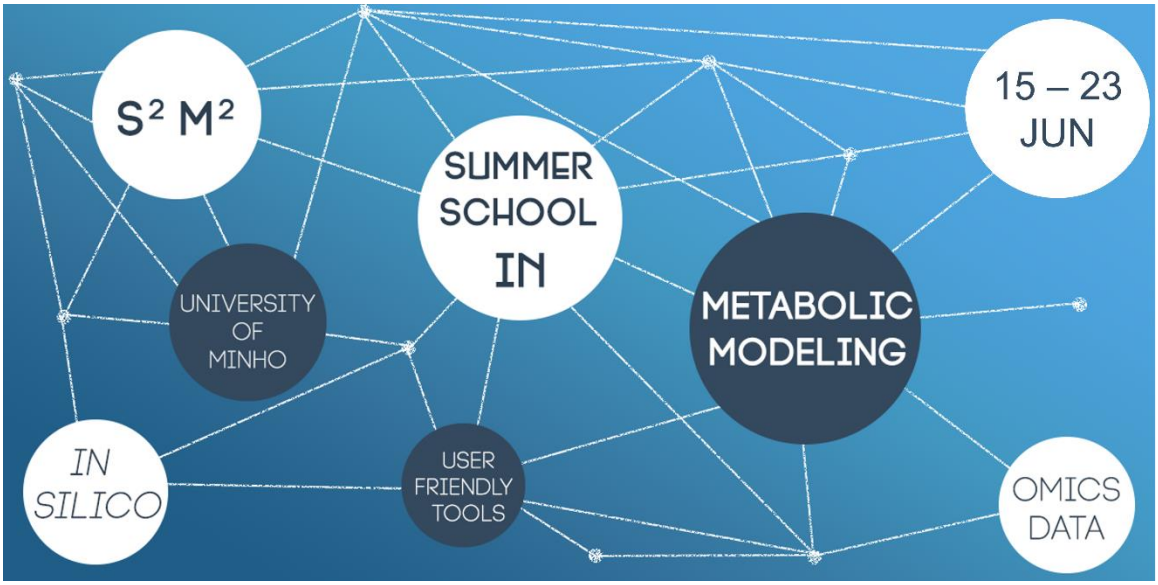
S2M2 sessions software requirements



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List of requirements regarding the following modules:

1. Hands-on in Python;
2. Flux analysis and Constraint-based modeling
3. Phenotype prediction
4. Strain optimization & Metabolic Engineering
5. Metabolic models, Machine learning & Omics data

Table of Contents

Requirements for S2M2

For this part of the S^2M^2, you will be required to have Python and CPLEX installed, alongside the required packages. This will be a guideline for the installation process. If you run into some issues when following this guide, please contact us.

Software needed:

- **Conda/Miniconda**
  - **https://docs.conda.io/en/latest/miniconda.html** here you can download the adequate installer for your operating system (OS).
  - **https://conda.io/projects/conda/en/latest/user-guide/install/index.html** in this link, follow the adequate instructions for the adequate OS in the section "Regular Installation". We advise you to keep selecting the defaults.
- **CPLEX Optimizer**
  - Use this link https://academic-prod.c8f8f055.public.multi-containers.ibm.com/a2mt/email-auth to sign up. You should use youracademic email and fill the small form. Validate your account with the email sent. After the validation is complete, go to https://www.ibm.com/analytics/cplex-optimizer and click on ***Access free academic edition***, on this link https://www.ibm.com/academic/technology/data-science scroll and click on ***Software***, look for ***ILOC CPLEX Optimization Studio***, click on register or login again and if you are logged in, it will refresh the page and generate a new link with ***Download ->*** on the samespot. Click on it and it will redirect you to a download page. Here, click on the Button with***HTTP*** on it and the select the adequate version of the CPLEX for your OS (and agree withthe terms). The windows file has 719MB, the LINUX one has 635 and the OSX one has

849MB. Save the location where you download the installer, since you will be needing it later.

Creating an environment in Conda/Miniconda:

If you are on Windows, use the search function in the windows start menu and search for “Anaconda” and open the “Anaconda Prompt” shortcut and it should open a terminal like the one presented below.

Figure 1 - How it should look like in Windows

For MacOS and Linux users, open a terminal and type “conda” and it should display a list of help functions like the picture below.

```
(base) [                                    ~]$ conda
usage: conda [-h] [-V] command ...

conda is a tool for managing and deploying applications, environments and packages.

Options:

positional arguments:
  command
    clean        Remove unused packages and caches.
    compare      Compare packages between conda environments.
    config       Modify configuration values in .condarc. This is modeled after the git config command. Writes to the user
                 .condarc file (/home/jorgemlferreira/.condarc) by default.
    create       Create a new conda environment from a list of specified packages.
    help         Displays a list of available conda commands and their help strings.
    info         Display information about current conda install.
    init         Initialize conda for shell interaction. [Experimental]
    install      Installs a list of packages into a specified conda environment.
    list         List linked packages in a conda environment.
    package      Low-level conda package utility. (EXPERIMENTAL)
    remove       Remove a list of packages from a specified conda environment.
    uninstall    Alias for conda remove.
    run          Run an executable in a conda environment. [Experimental]
    search       Search for packages and display associated information. The input is a MatchSpec, a query language for conda
                 packages. See examples below.
    update       Updates conda packages to the latest compatible version.
    upgrade      Alias for conda update.

optional arguments:
  -h, --help     Show this help message and exit.
  -V, --version  Show the conda version number and exit.
```

Figure 2 - How it should look like in MacOS/Linux

Creating the specific environment for both modules

Now, you will need to create the environment where you will install all the packages necessary and this part is the same for all OS. On your terminal, type ***conda create -n s2m2 python=3.7*** and press **ENTER**. This will begin to prepare the installation and when prompted with **Proceed ([y]/n)?** type **y** and press **Enter**.

```
The following packages will be downloaded:

    package                    |            build
    ---------------------------|-----------------
    _libgcc_mutex-0.1          |             main           3 KB
    _openmp_mutex-4.5          |            1_gnu          22 KB
    ca-certificates-2021.5.25  |       h06a4308_1         112 KB
    certifi-2021.5.30          |   py37h06a4308_0         139 KB
    ld_impl_linux-64-2.35.1    |       h7274673_9         586 KB
    libgcc-ng-9.3.0            |       h5101ec6_17        4.8 MB
    libgomp-9.3.0              |       h5101ec6_17        311 KB
    libstdcxx-ng-9.3.0         |       hd4cf53a_17        3.1 MB
    openssl-1.1.1k             |       h27cfd23_0         2.5 MB
    pip-21.1.3                 |   py37h06a4308_0         1.8 MB
    python-3.7.10              |       h12debd9_4        44.0 MB
    setuptools-52.0.0          |   py37h06a4308_0         710 KB
    sqlite-3.36.0              |       hc218d9a_0         990 KB
    ------------------------------------------------------------
                                           Total:        59.0 MB

The following NEW packages will be INSTALLED:

  _libgcc_mutex      pkgs/main/linux-64::_libgcc_mutex-0.1-main
  _openmp_mutex      pkgs/main/linux-64::_openmp_mutex-4.5-1_gnu
  ca-certificates    pkgs/main/linux-64::ca-certificates-2021.5.25-h06a4
  certifi            pkgs/main/linux-64::certifi-2021.5.30-py37h06a4308_
  ld_impl_linux-64   pkgs/main/linux-64::ld_impl_linux-64-2.35.1-h72746
  libffi             pkgs/main/linux-64::libffi-3.3-he6710b0_2
  libgcc-ng          pkgs/main/linux-64::libgcc-ng-9.3.0-h5101ec6_17
  libgomp            pkgs/main/linux-64::libgomp-9.3.0-h5101ec6_17
  libstdcxx-ng       pkgs/main/linux-64::libstdcxx-ng-9.3.0-hd4cf53a_17
  ncurses            pkgs/main/linux-64::ncurses-6.2-he6710b0_1
  openssl            pkgs/main/linux-64::openssl-1.1.1k-h27cfd23_0
  pip                pkgs/main/linux-64::pip-21.1.3-py37h06a4308_0
  python             pkgs/main/linux-64::python-3.7.10-h12debd9_4
  readline           pkgs/main/linux-64::readline-8.1-h27cfd23_0
  setuptools         pkgs/main/linux-64::setuptools-52.0.0-py37h06a4308_
  sqlite             pkgs/main/linux-64::sqlite-3.36.0-hc218d9a_0
  tk                 pkgs/main/linux-64::tk-8.6.10-hbc83047_0
  wheel              pkgs/main/noarch::wheel-0.36.2-pyhd3eb1b0_0
  xz                 pkgs/main/linux-64::xz-5.2.5-h7b6447c_0
  zlib               pkgs/main/linux-64::zlib-1.2.11-h7b6447c_3


Proceed ([y]/n)? y
```

Figure 3 - Example of how the prompt is presented

It will begin to download and install some important packages and in the end it should look like this.

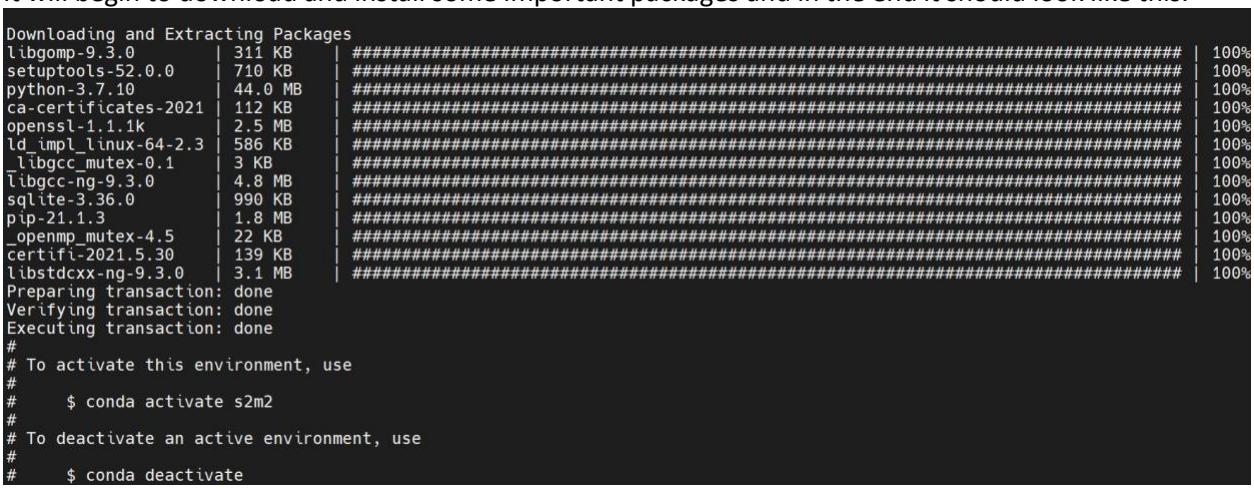

Figure 4 - End of installation of python 3.7

What this does is creating a separate installation of Python where you will have a different Python version from your OS (especially on MacOS and Linux). Still in the terminal, type ***conda activate s2m2*** (instead of ***conda***, you may have to type ***source***; if that is the case, every time from now on that you will have to type ***conda***, type ***source*** instead) and you should have changed to the correct environment. The beginning of your terminal should look like this.

Figure 5 - Example of the activation of the correct environment. In your terminal ,(s2m2) should be present

Whenever you close the terminal, and turn it on again, you will always have to activate the s2m2 environment. Inside of (XXXX) is the name of the current environment you are working on.

Installing the required packages

Packages from pip

Now, we will install the necessary packages to use in these modules. With the ***s2m2*** environment activated, you have to type ***pip install troppo mewpy jupyter escher***. In the end of the installation process, it should display something like what is shown in the picture below.

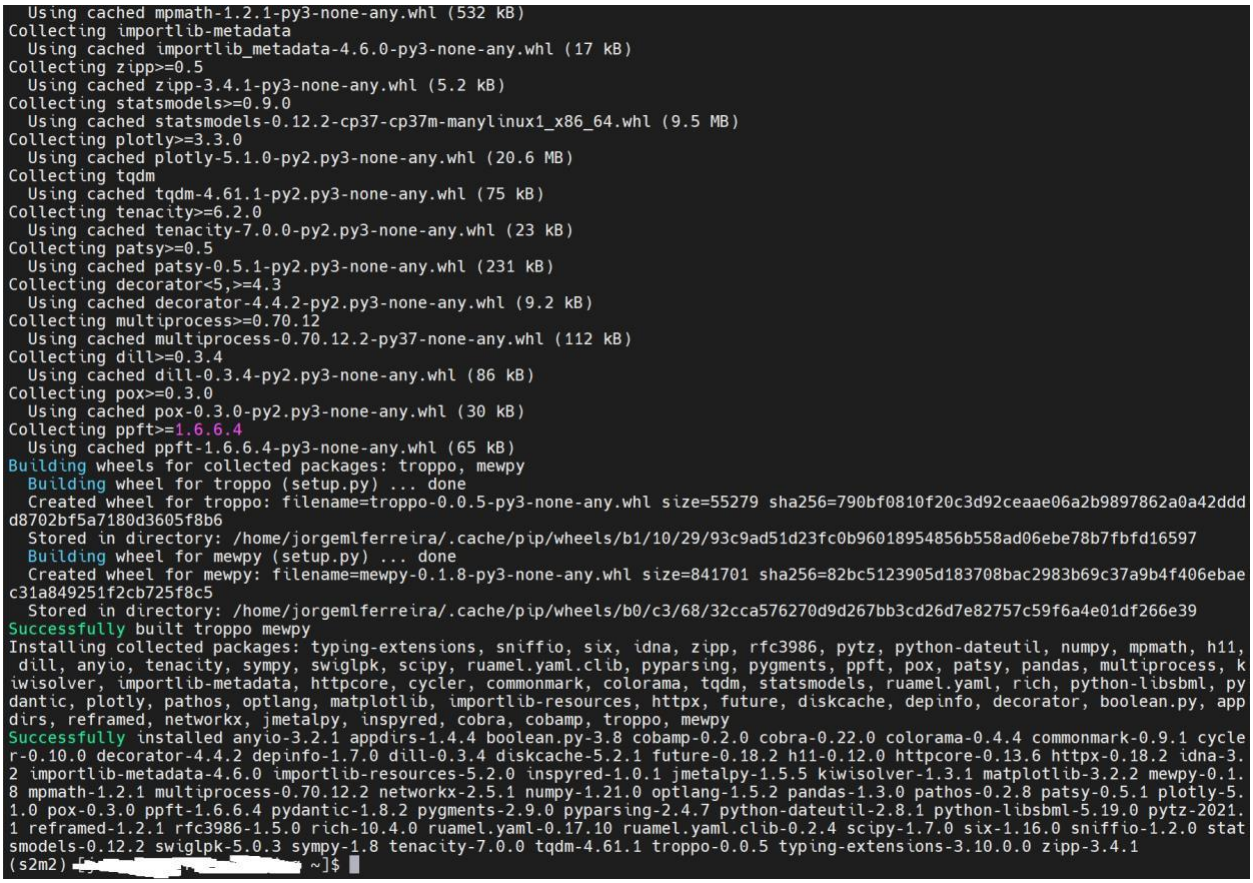

Figure 6 - Example of a successful installation of the required packages

Just to verify if everything is working, type ***python*** on the terminal and press ***Enter***. If you see ***>>>*** before you type anything, you are now on the console of Python. To check if everything is correctly installed, type:

import mewpy, troppo, jupyter, escher, cobra

And then press ***Enter***. If the next line is ***>>>*** and with no text before, it means the packages were imported correctly. Type ***exit()*** and then press ***ENTER*** to exit python and go back to the terminal.

Packages from Git

The ***etfl*** package is also necessary, but it is not present in ***pip***. To install it, you will need to clone the repository. Since Windows does not have a built-in Git installed, we will have two different approaches to install this, for Windows and for MacOS/LINUX.

If you are on a Windows system, download this .zip from the link https://github.com/EPFL-

LCSB/etfl/archive/refs/heads/master.zip . Extract the content of the .zip for a folder and save the location of it.

If you are on a MacOS/LINUX system, with your terminal open, type ***git clone https://github.com/EPFL-LCSB/etfl.git /path/to/etfl*** where ***/path/to/etfl*** is the location where the folder containing the code for the ***eftl*** package is kept.

From here on, it will be the same for both operating systems.

In the terminal, type ***cd /path/to/eftl*** (where you unzip or made a clone of git) and press ***ENTER***. With the s2m2 conda environment activated, type ***python setup.py install*** and it should be installed with no problem.

To check if it is correctly installed, type ***python*** and press ***ENTER***. It should open the Python console. Then type ***import eftl*** and if there are no errors, the package is successfully installed. Type ***exit()*** and press ***ENTER*** to exit the python console.

Installing CPLEX

For installing the CPLEX in all available OS, please follow the instruction present in this link https://www.ibm.com/docs/en/icos/20.1.0?topic=2010-installing-cplex-optimization-studio . If you find any trouble with the installation of the CPLEX, please contact us.

Installing CPLEX for Python

With the ***s2m2*** conda environment activated, go to yourCplexhome(depends on the OS you use)/python/PYTHON_VERSION/OS and there it should be a ***setup.py*** file; go to that folder in the terminal and then ***python setup.py install***. Agree with every step and CPLEX should be available with the python on your conda environment. To test this, type ***python*** on your terminal and the ***ENTER***. Then, type ***import cplex*** and check if there are no errors. If not, type ***exit()*** and then press ***ENTER*** to exit python.

Opening a Jupyter notebook to code

Move your current folder to the one where you have your working files for the S^2M^2 files for this. An example could be in your home/desktop in your terminal. After this, type ***jupyter-notebook*** on your terminal and then press ***ENTER***. It automatically should open your browser (if you are working on your own PC and not in a server, per example). It should open a tab like this:

Figure 7 - Example of a jupyter notebook interface

If for some reason you are not able to get this 1st try on your browser, copy either the localhost or 127.0.0.1 links present in your terminal and paste them in your browser.

Figure 8 - Links to open the jupyter notebook

Finally, to open an interface where you can program, click on new on the top right corner and select the Python 3 version.

Figure 9 - Steps to open a jupyter notebook

It will open a new tab and you are ready to go.

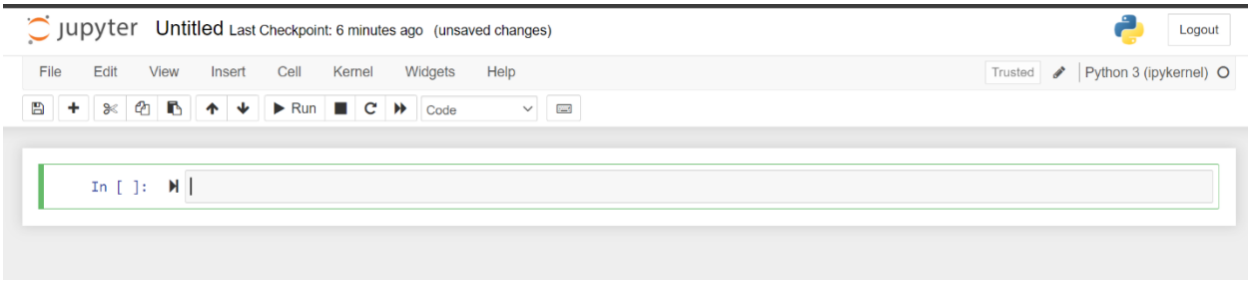

Figure 10 - Example of a jupyter notebook

If you have any doubts about this, please contact someone in the organization to help you throughout this setup.