**Install and Use the Growth-Coupling Suite in a Virtual Environment**

Requirements:

* Eligibility for a Gurobi solver license
* Clone or downloaded distribution of the Growth-Coupling Suite (GCS)

**Virtual Environments using Anaconda/conda**

Using an Anaconda distribution for creating a virtual environment is recommended if you do not have experience in Python and do not have a preinstalled Python version.

1. Install an Anaconda distribution
   1. Download the installer for the free individual edition for your system (<https://www.anaconda.com/products/individual>)
   2. Install Anaconda via the installer
   3. Comes with a Python distribution and preinstalled packages such as Jupyter Lab/Notebook.
2. Install the latest Gurobi solver
   1. Go to [https://www.gurobi.com/](https://www.gurobi.com/%20), register and, login
   2. Download and install the latest Gurobi solver version (9.5 tested)
   3. In your Gurobi account, get a free academic license
   4. Activate your license
3. Create and activate a [virtual conda environment](https://towardsdatascience.com/getting-started-with-python-environments-using-conda-32e9f2779307)
   1. Open the Anaconda prompt (as an administrator)

*In Windows, type “Anaconda Prompt” into the search bar*

* 1. Create a virtual environment with Python 3.9

conda info --envs

conda create --name env\_gcs python=3.9

* 1. (Optional) Check the virtual environment *env\_gcs* was created
  2. Activate the virtual environment

conda activate env\_gcs

* 1. The command line should now start with *(env\_gcs)*

1. Install the Growth-Coupling Suite within the virtual environment
   1. Make sure the virtual environment is activated
   2. Install [equilibrator-api](https://equilibrator.readthedocs.io/en/latest/index.html) for creating heterologous reaction databases

pip install equilibrator-api

To complete the equilibrator installation execute the following command

python -c "from equilibrator\_api import ComponentContribution; cc = ComponentContribution()"

**Important**: Install equilibrator-api before installing the growth-coupling-suite

* 1. (Optional) Install [COBRApy](https://cobrapy.readthedocs.io/en/latest/) (may be automatically installed with the GCS -> f)

pip install cobra==0.25.0

**Info:** For compatibility reasons the cobrapy version 0.25.0 (and with it a corresponding optlang version) is installed

* 1. (Optional) Install the [Python API for the Gurobi Solver](https://support.gurobi.com/hc/en-us/articles/360044290292-How-do-I-install-Gurobi-for-Python-) (may be automatically installed with the GCS -> f)

pip install gurobipy==9.5.2

**Info:** Compatibility with the growth-coupling suite was tested for gurobipy version 9.5.2

* 1. In the Anaconda prompt, navigate to the folder with the GCS clone (the folder should contain the setup.py)
  2. Install the GCS via the setup.py file

python setup.py develop

1. Install Jupyter Notebook/Lab for using the prepared GCS workflows

*Option 1*

* 1. Open the Anaconda Navigator
  2. In dropdown menu *Applications on* select the previously created virtual environment *env\_gcs*
  3. Press *Install* on the Jupyter Notebook window

*Option 2*

* 1. Make sure the virtual environment is activated (c.f. 3)

pip install jupyter

* 1. Install Jupyter Notebook via pip

or Jupyter Lab

pip install jupyterlab

1. Test the GCS
   1. Open the Anaconda Navigator
   2. In dropdown menu *Applications on* select the previously created virtual environment *env\_gcs*
   3. Open Jupyter Notebook or Lab

*Option 1*

* 1. In Jupyter navigate to the folder of the GCS distribution and further the *example* folder
  2. Open *conduct\_gcOpt\_optimization.ipynb*
  3. Run the script
  4. If successful, a folder named *results* was created with an Excel file *gcOpt\_summary\_result.xlsx* summarizing the GCS results

*Option 2*

* 1. Run the short course script(s)

**Virtual Environments using virtualenv**

1. Install a Python 3.8 release. We recommend Python 3.8.10. If you already have and work with Python 3.8 on your system you don’t need to do this.
   1. Download and install Python 3.8.10 release for your OS (<https://www.python.org/downloads/)>. For detailed instructions have a look at <https://python.land/python-tutorial>

**Info 1:** Python 3.8 is installed to ensure compatibility with cobrapy 0.20.0 (see below).

**Info 2:** Make sure you know the path to the installation folder of Python 3.8. We will need to specify the path to create a virtual environment. In the following, we will assume the Python 3.8 distribution is found at *C:\Python\Python38* (Windows). Please adapt to your OS.

1. On Windows, make sure the path to the Python installation folder is added to the Windows Path variable (<https://geek-university.com/python/add-python-to-the-windows-path/)>. If you followed 1) and this is the only Python installation add the path *C:\Python\Python38.* You can also use another existent Python 3 installation. Also add the path to the folder *Scripts* in the Python installation folderto the Windows Path (*C:\Python\Python38\Scripts*).
2. Install the *virtualenv* package
   1. In the command prompt (e.g. cmd on Windows) type

pip install virtualenv

1. Create a new folder where the virtual environment will be installed. You can choose an arbitrary location for this folder. Navigate to this folder in the command prompt.
2. Create a virtual environment named *py38\_gcs\_env* based on Python 3.8 using *virtualenv*

virtualenv -p C:\Python\Python38\python.exe py38\_gcs\_env

**Info**: The virtual environment *py38\_gcs\_env* will be installed in the current directory using the Python distribution installed at *C:\Python\Python38.* Make sure that the basis of the virtual environment is Python 3.8.

1. Activate the virtual environment

py38\_gcs\_env\Scripts\activate

* 1. On Windows
  2. On Mac

py38\_gcs\_env/bin/activate

**Info**: *(py38\_gcs\_env)* is now added to the prompt

1. Follow 4) and 5) in the previous section “Virtual Environments using Anaconda/conda” to install the Growth-coupling Suite using the current prompt.

**Info**: Install Jupyter notebook via

pip install jupyter

And open it via

jupyter notebook

1. Test the GCS according to 6) in the section “Virtual Environments using Anaconda/conda”