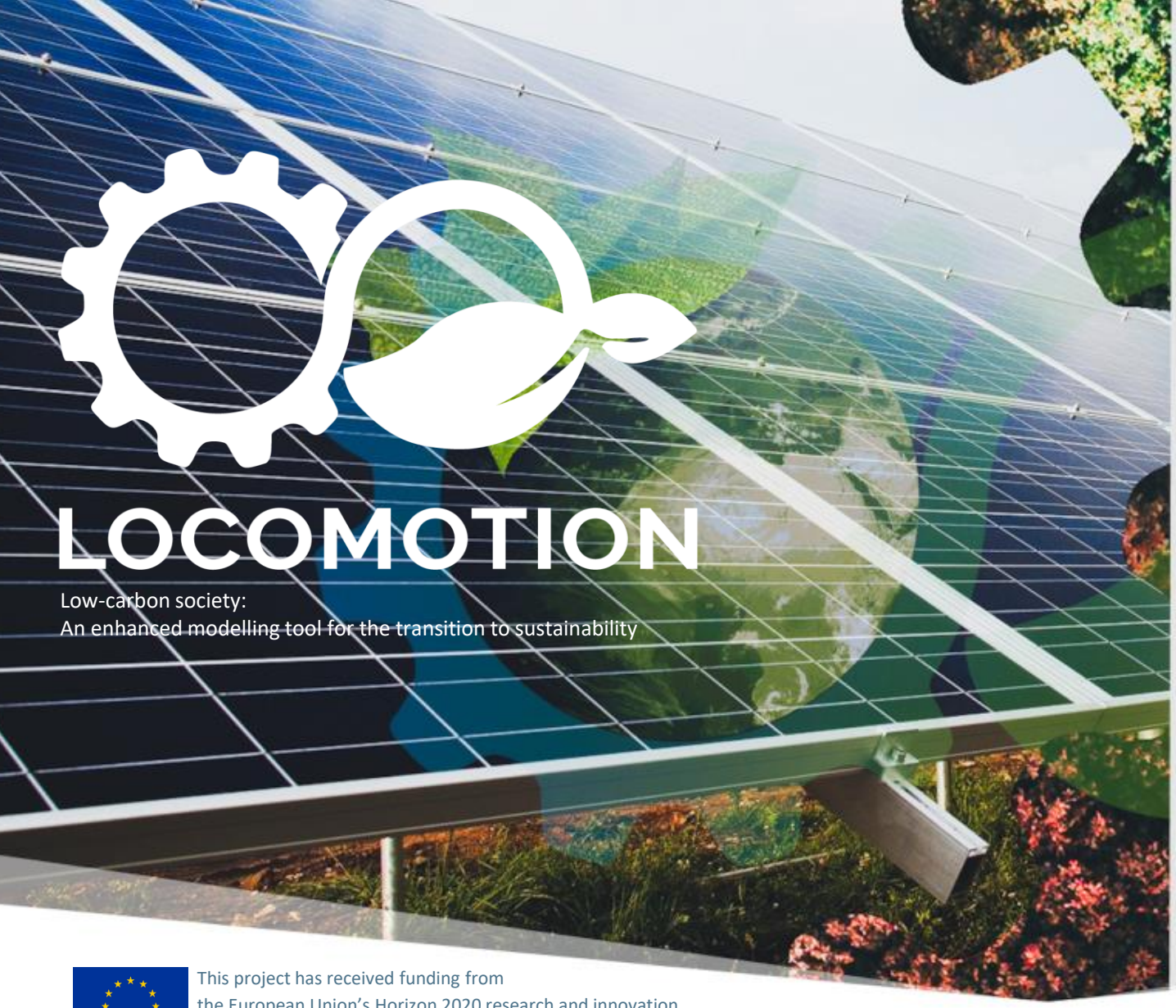

LOCOMOTION

Low-carbon society:
An enhanced modelling tool for the transition to sustainability

The pywiliam model

Simulating WILIAM using a Python model

LOCOMOTION project

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 821105.

6.1 Contents

6.2 Main features of pywiliam

WILIAM model v1.1 translated to **Python** using the PySD library (https://github.com/SDXorg/pysd)

PySD
Simulating System Dynamics Models in Python

Fully open source (MIT)

JOSS
The Journal of Open Source Software

Multiplatform (GNU/Linux, Mac, Windows, etc)

PySD: System Dynamics Modeling in Python

Eneko Martin-Martinez [1*], **Roger Samsó** [1*¶], **James Houghton** [2], and **Jordi Solé** [1,3]

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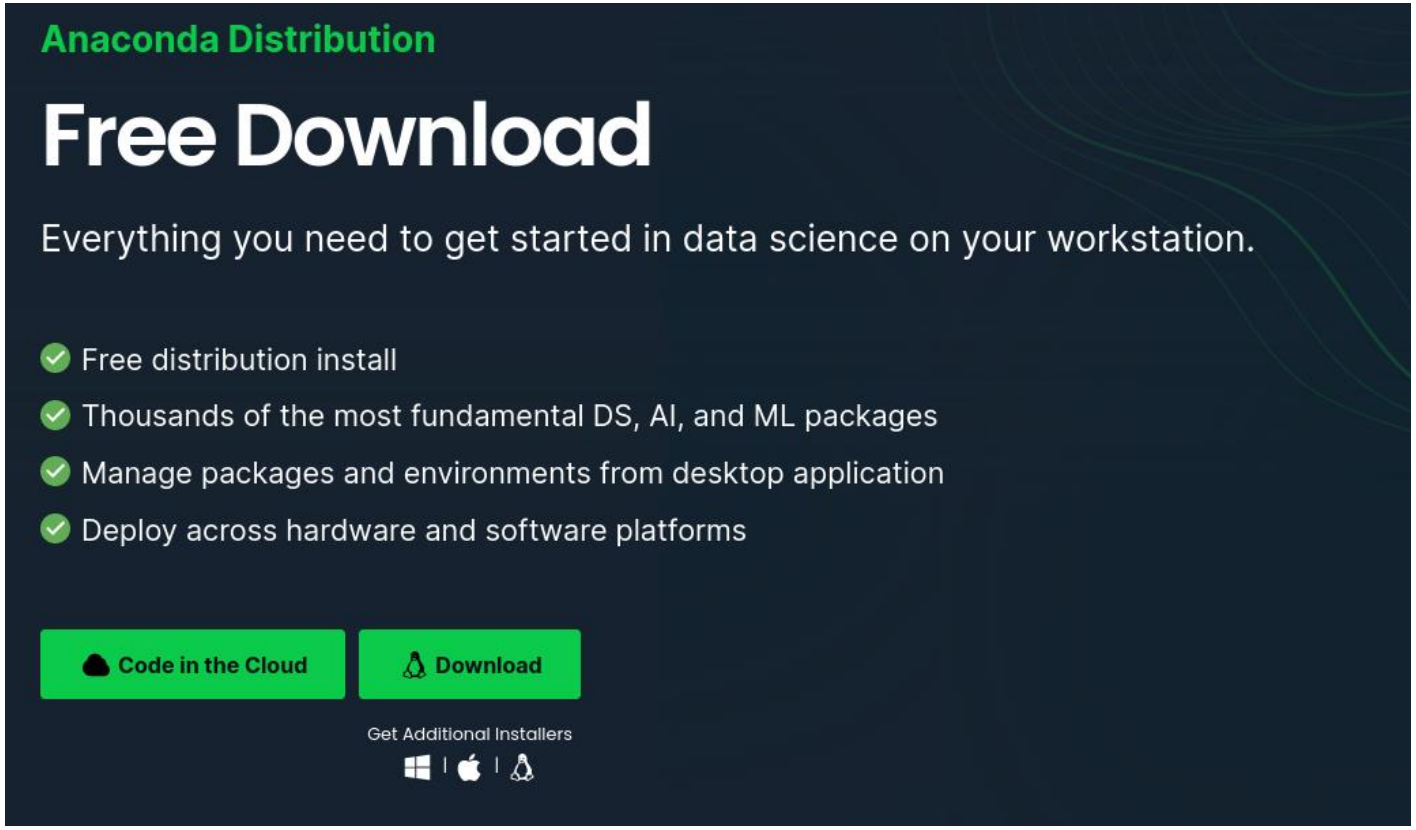
DOI: 10.21105/joss.04329

6.3 Installing Anaconda Python

https://www.anaconda.com/download



6.4 Opening Anaconda prompt and moving to the pywiliam directory

Anaconda Powershell Prompt

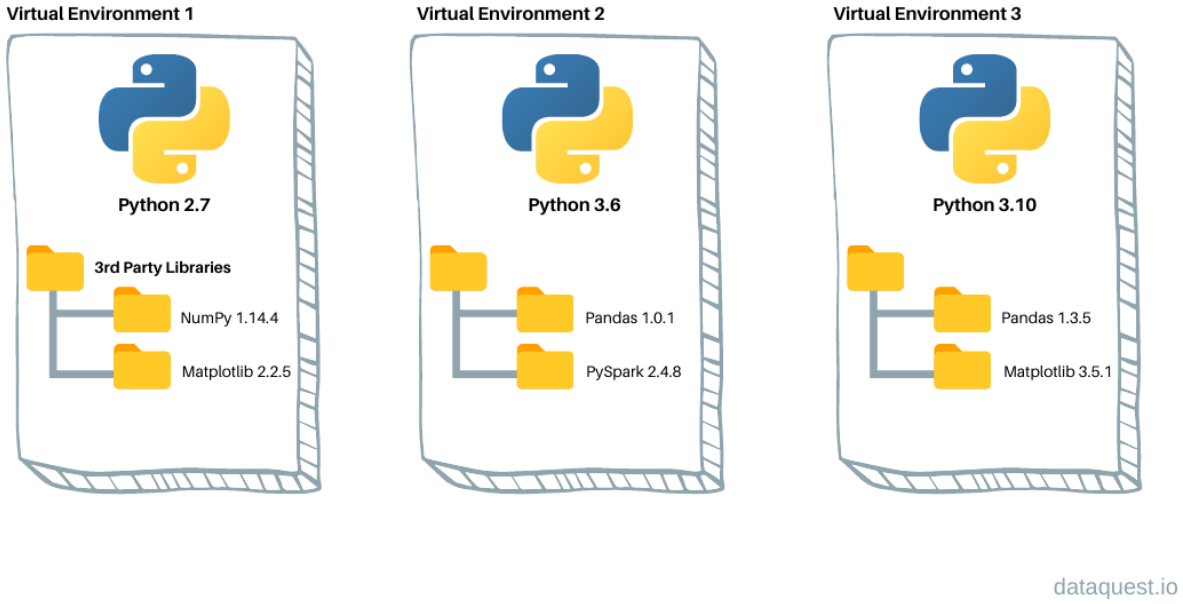
```
(base) PS C:\Users\ivaram> D:
(base) PS D:\> cd DATA_3
(base) PS D:\DATA_3> cd pywiliam-main
(base) PS D:\DATA_3\pywiliam-main> conda config --add channels conda-forge
(base) PS D:\DATA_3\pywiliam-main> conda create --name wiliam python=3.11 --file requirements.txt
Collecting package metadata (current_repodata.json): done
Solving environment: done


==> WARNING: A newer version of conda exists. <==
  current version: 4.8.3
  latest version: 23.10.0

Please update conda by running

    $ conda update -n base conda


WARNING conda.gateways.disk.delete:unlink_or_rename_to_trash(140): Co
s\boost-cpp-1.78.0-h9f4b32c_1.tar.bz2.  Please remove this file manua
WARNING conda.gateways.disk.delete:unlink_or_rename_to_trash(140): Co
s\boost-cpp-1.78.0-h9f4b32c_1\Library\bin\boost_log_setup.dll.  Pleas
```

Anaconda Powershell Prompt

```
 to free file handles)

## Package Plan ##

  environment location: C:\Users\ivaram\.conda\envs\wiliam

  added / updated specs:
    - dacite
    - dask
    - matplotlib
    - netcdf4
    - pysd[version='>=3.10']
    - python=3.11
    - tk


The following packages will be downloaded:

    package                    |            build
    ---------------------------|-----------------
    aws-c-auth-0.7.5           |       hf425296_2          96 KB  conda-forge
    aws-c-cal-0.6.9            |       h6f45060_0          54 KB  conda-forge
    aws-c-common-0.9.5         |       hcfcfb64_0         214 KB  conda-forge
    aws-c-compression-0.2.17   |       h6f45060_5          22 KB  conda-forge
    aws-c-event-stream-0.3.2   |       h65f5141_5          54 KB  conda-forge
    aws-c-http-0.7.13          |       h4076b5e_9         176 KB  conda-forge
    aws-c-io-0.13.35           |       he032580_7         155 KB  conda-forge
    aws-c-mqtt-0.9.8           |       he63eff1_1         154 KB  conda-forge
    aws-c-s3-0.3.22            |       h40b9648_1          84 KB  conda-forge
    aws-c-sdkutils-0.1.12      |       h6f45060_4          51 KB  conda-forge
```

6.5 Creating a virtual environment with conda

What are Python virtual environments and why we need them?



6.5 Creating a virtual environment with conda

Add conda-forge channel:

```
conda config --add channels conda-forge
```

To create a virtual environment using conda, run:

```
conda create --name wiliam python=3.11 --file requirements.txt
```

The previous command created a virtual environment named `wiliam`. To activate it, run:

```
conda activate wiliam
```

To run the wiliam model, you need to be inside the virtual environment, but if you want to exit it, run:

```
conda deactivate
```

6.6 Running a simulation

A wiliam simulation using default parameters can be run by simpply typing:

```
python run.py
```

```
Anaconda Powershell Prompt

(wiliam) PS D:\DATA_3\pywiliam> python run.py


Simulation parameters:
- Scenario file: scenario_parameters.xlsx
- Initial time: 2005.0
- Final time: 2050.0
- Simulation time step: 0.25 years (91.25 days)
- Results folder: D:\DATA_3\pywiliam\results
Time:  0:35:44 [##################################################################################################]100%
Results stored in D:\DATA_3\pywiliam\results\results_scenario_parameters_2005_2050_0.25.nc
INFO - Thu, 09 Nov 2023 15:50:30, 225: Total simulation time: 38.48 minutes
(wiliam) PS D:\DATA_3\pywiliam>
```

Additionally, if the user only wants to play with scenario parameters, a good initialisation speedup may be achieved by loading the model parameters from a binary file, as follows:

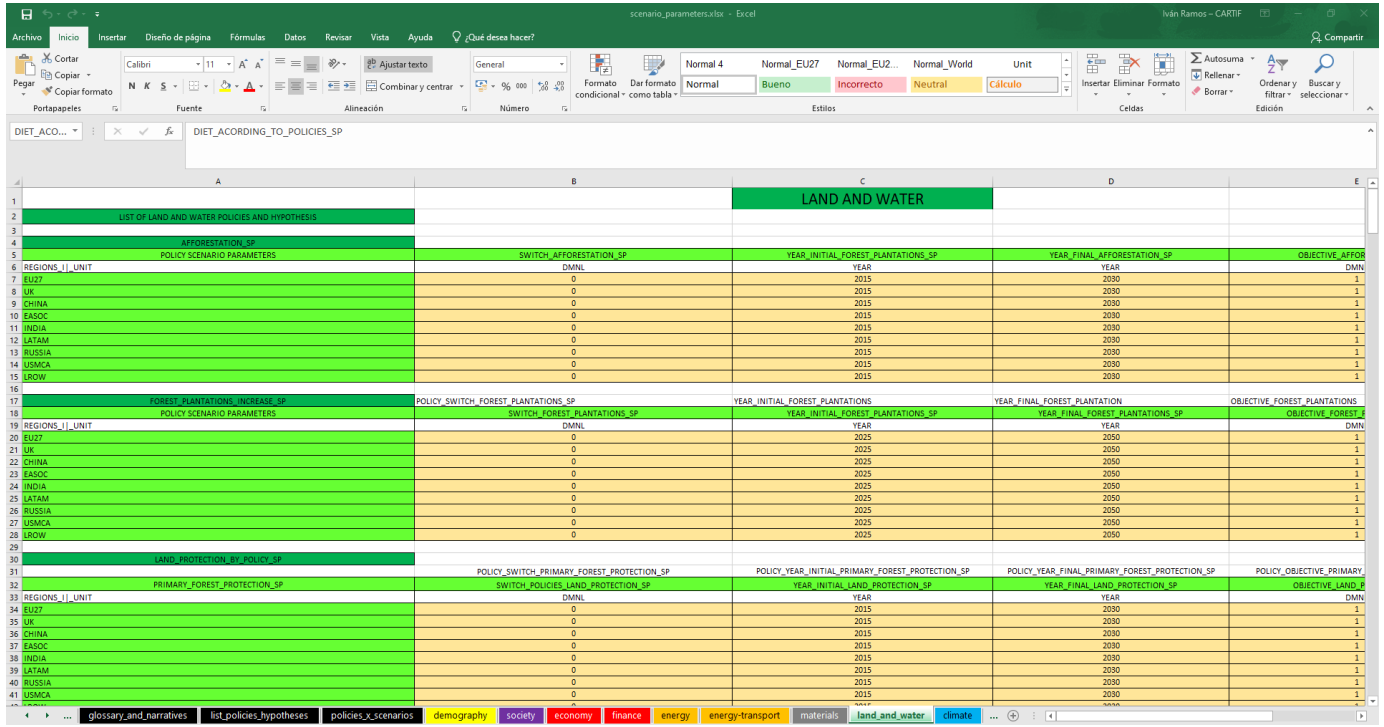
```
python run.py -e wiliam/model_parameters/model_parameters.nc
```

6.7 Creating and simulating a new scenario

To create a new scenario, duplicate the scenario_parameters.xlsx file and give it a descriptive name (eu_green_deal.xlsx).

To run a simulation with the newly created scenario, run:

```
python run.py -x eu_green_deal
```



6.8 Additional configurations

```
python run.py -h
```

```
usage: usage: pywiliam [-h] [-v] [-n FILE] [-e FILE] [-p] [-c SHEET] [-x FILE] [-b] [-s] [-F VALUE] [-T VALUE] [-S VALUE]
               [--missing-values {warning,raise,ignore,keep}]
               [variable=new_value ...] [variable:initial_value ...]

WILIAM model

positional arguments:
  variable=new_value    redefine the value of variable with new value.variable must be a model component, new_value can be
                        a float or a a list of two list
  variable:initial_value
                        redefine the initial value of variable.variable must be a model stateful element, initial_value
                        must be a float

options:
  -h, --help            show this help message and exit
  -v, --version         show program's version number and exit
  -n FILE, --fname FILE
                        name of the results file, default is results_{scenario sheet}_{initial time}_{final time}_{time
                        step}.csv
  -e FILE, --externals FILE
                        path to the netCDF file where the external objects are stored
  -p, --plot            opens the plot gui after simulation
  -c SHEET, --scen SHEET
                        scenario file path
  -x FILE, --export FILE
                        export stateful objects states to a pickle at the end of the simulation
  -b, --headless        headless mode (only CLI, no GUI)
  -s, --silent          silent mode. No user input will be required during execution. Usefulwhen running batch simulations

model arguments:
  Modify model control variables.

  -F VALUE, --final-time VALUE
                        modify final year of the simulation, default is 2050.0
  -T VALUE, --time-step VALUE
                        modify time step (in years) of the simulation, default is 0.25
  -S VALUE, --saveper VALUE
                        modify time step (in years) of the output, default is 1.0 year

warning and errors arguments:
  Modify warning and errors management.

  --missing-values {warning,raise,ignore,keep}
                        exception with missing values, 'warning' (default) shows a warning message and interpolates the
                        values, 'raise' raises an error, 'ignore' interpolates the values without showing anything, 'keep'
                        keeps the missing values
```

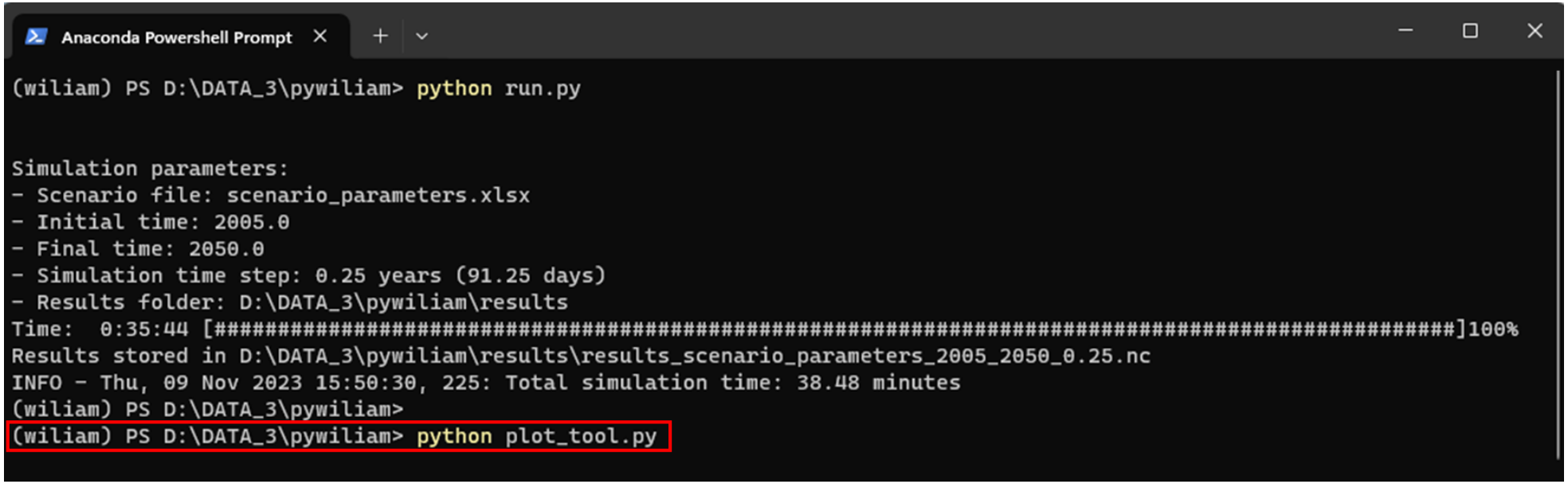
6.9 Plotting the results

If the `-p` argument is passed to the CLI, a graphical user interface will load automatically after the simulation ends, which lets the users plot the results:

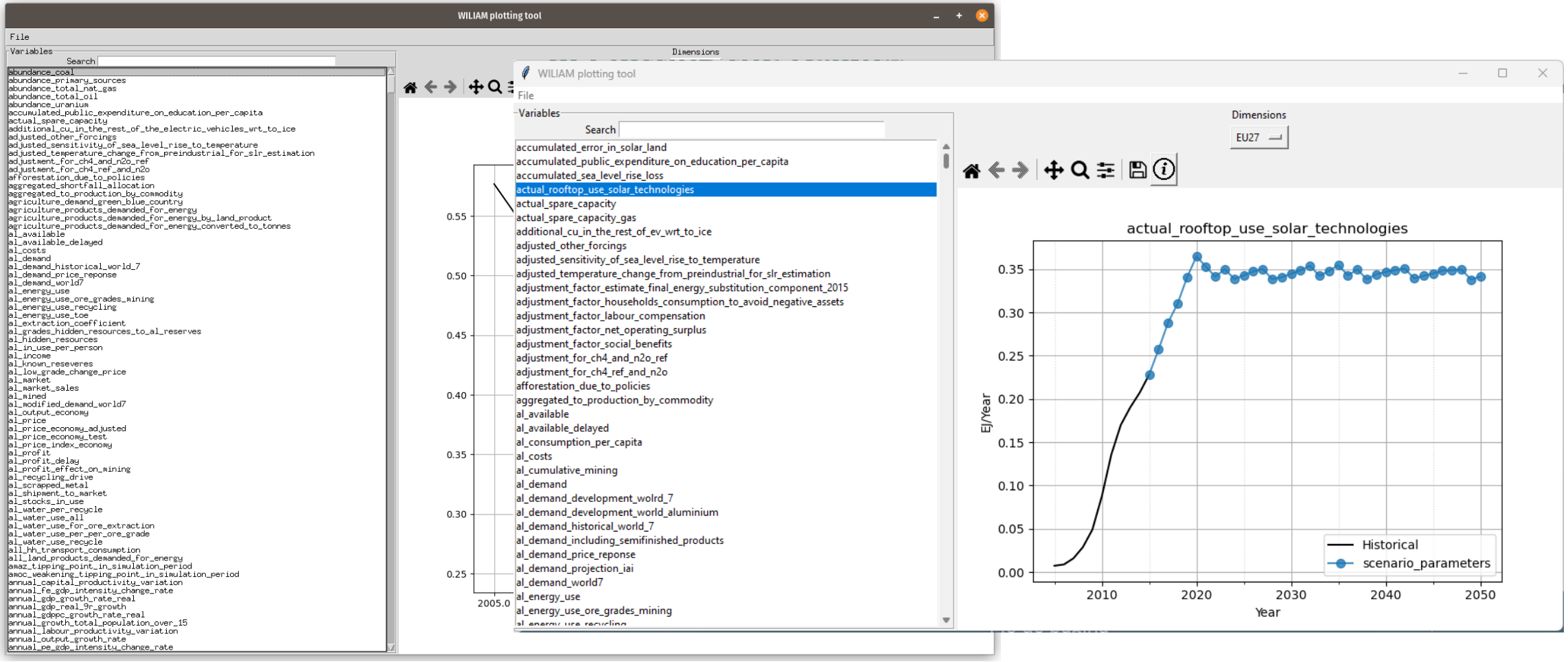
```
python run.py -h
```

Alternatively, the plot tool may be launch in standalone mode, by running:

```
python plot_tool.py
```



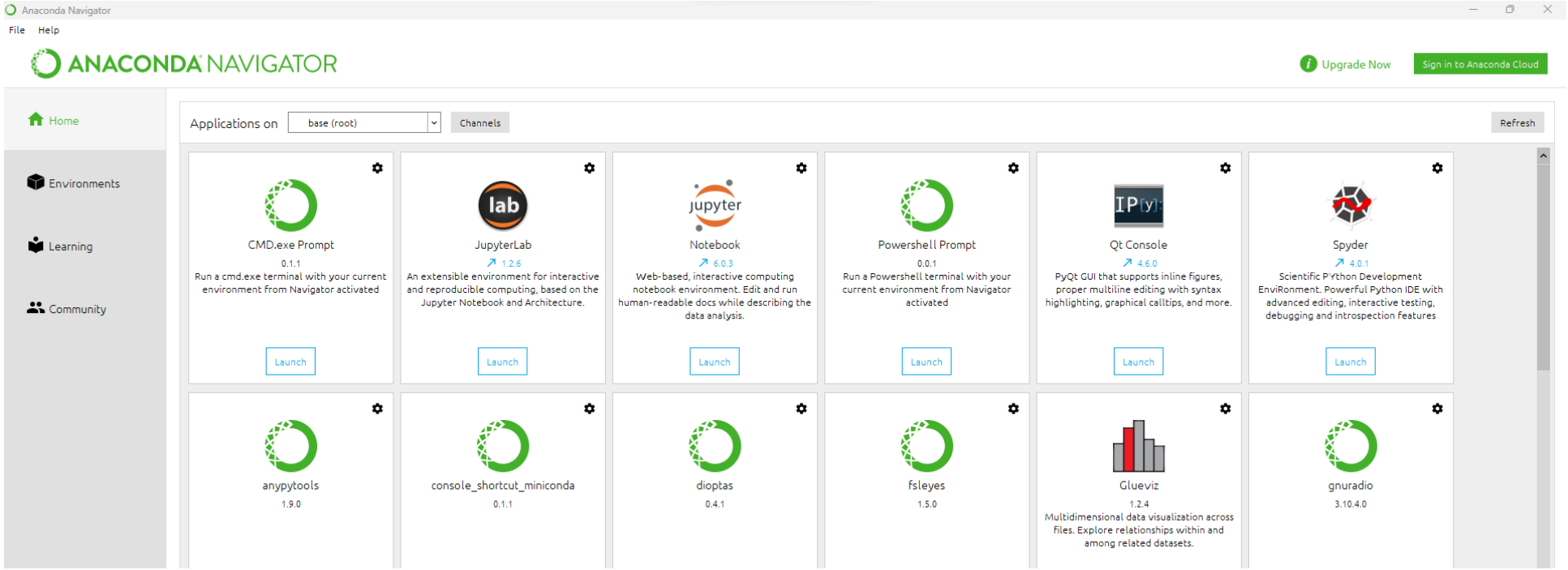
6.9 Plotting the results



6.10 Additional tools (exporting from netCDF to csv)

Use **Jupyter Notebook**

- Launch Anaconda
- Create a New Environment
- Install libraries and open the environment



6.10 Additional tools (exporting from netCDF to csv)

Managing and exporting datasets from .nc files

By following this tutorial, you should be able to open a nc file, visualize the parameters and variables stored on it and export some of them to a tab or csv file.

In [ ]:
```
import pysd
from pysd.tools.ncfiles import NCFile
import pandas as pd
import warnings

pd.set_option('display.max_row', None)
warnings.filterwarnings('ignore')
```

WARNING: To use this script, you must be using PySD 3.8 or newer, and the netCDF4 and dask Python libraries must be installed in your environment.

In [ ]:
```
pysd.__version__
```

In [ ]:
```
# folder where the nc file is lo
# no need to change this one, un  u moved the nc file to a different folder
results_folder = "../results/"
```

Configure exports paths

In [ ]:
```
# Put here the name of the nc file you want to export data from
simulation_results = "results_scenario_parameters_2005_2010_0.25.nc"
```

The exported data will be stored in the results folder in a tab file with the same name (i.e. results_scenario_parameters_2005_2010_0.25_export.tab)

6.10 Additional tools (exporting from netCDF to csv)

Managing and exporting datasets from .nc files

By following this tutorial, you should be able to open a nc file, visualize the parameters and variables stored on it and export some of them to a tab or csv file.

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import pandas as pd
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pd.set_option('display.max_row', None)
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```

WARNING: To use this script, you must be using PySD 3.8 or newer, and the netCDF4 and dask Python libraries must be installed in your environment.

In [ ]:
```
pysd.__version__
```

In [ ]:
```
# folder where the nc file is located
# no need to change this one, unless you moved the nc file to a different folder
results_folder = "../results/"
```

Configure exports paths

In [ ]:
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# Put here the name of the nc file you want to export data from
simulation_results = "results_scenario_parameters_2005_2010_0.25.nc"
```

The exported data will be stored in the results folder in a tab file with the same name (i.e. results_scenario_parameters_2005_2010_0.25_export.tab)

Define variables to export

Define here which model parameters or variables you wish to export.

You can choose any model variable (including inputs)

In [ ]:
```
# Modify this list
variables_to_export = ["total_water_demand_region", "total_mineral_supply"]
```