

Getting mercury to run locally

We will use a program called **mercury** to run the simulation locally on the computer. **mercury** is a convenient tool that converts our Python code into a web app.

Step 0: Logon to the computer

Username: .\Ircguest (note: backslash, not forward slash)

Password: (will be provided)

Step 1: Download the jupyter notebook **random-walk-2d-mercury.ipynb**.

On github:

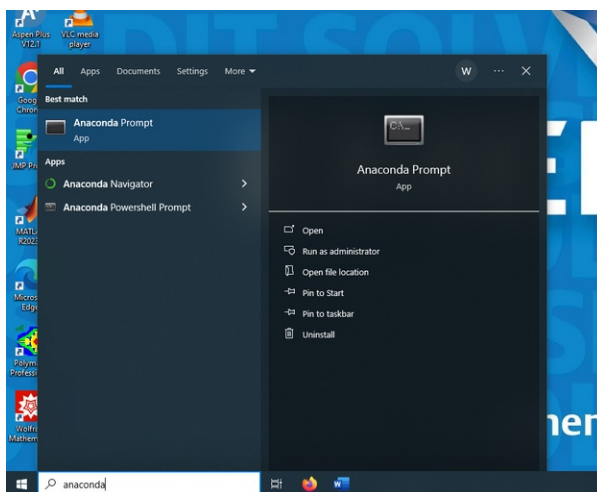
<https://github.com/wangmatgroup/outreach/tree/main/MITE/Su24-diffusion/random-walk-mercury>

On Google Drive:

<https://shorturl.at/uebUF>

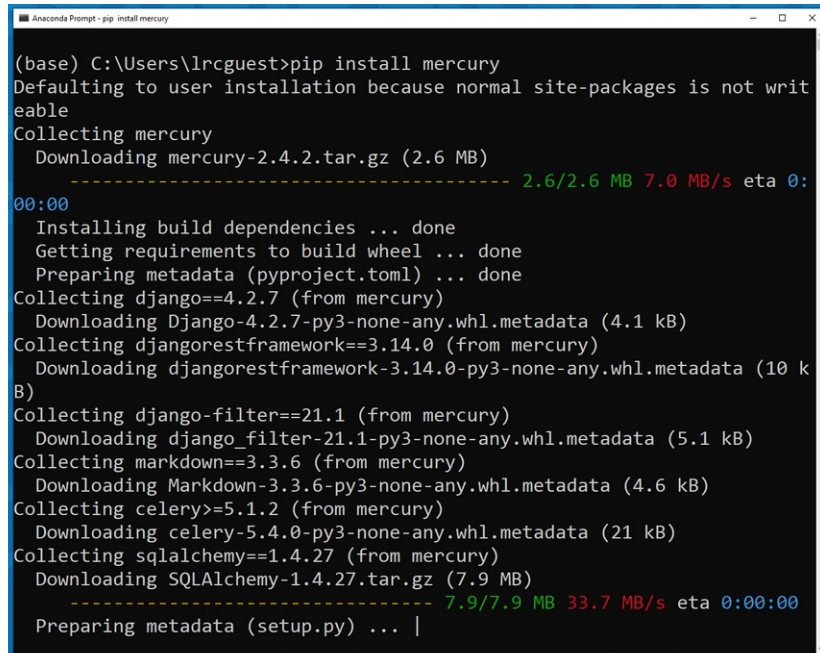
The notebook will automatically download to the **Downloads** folder.

Step 2: Open Anaconda Prompt. This will open a command window prompt.



Step 3: Download mercury through the command window prompt.

Type in **pip install mercury** and hit 'Enter.' You will see a lot of text generating; something like the following.



```

Anaconda Prompt - pip install mercury

(base) C:\Users\lrcguest>pip install mercury
Defaulting to user installation because normal site-packages is not writeable
Collecting mercury
  Downloading mercury-2.4.2.tar.gz (2.6 MB)
    ----- 2.6/2.6 MB 7.0 MB/s eta 0:00:00
Installing build dependencies ... done
Getting requirements to build wheel ... done
Preparing metadata (pyproject.toml) ... done
Collecting django==4.2.7 (from mercury)
  Downloading Django-4.2.7-py3-none-any.whl.metadata (4.1 kB)
Collecting djangorestframework==3.14.0 (from mercury)
  Downloading djangorestframework-3.14.0-py3-none-any.whl.metadata (10 kB)
Collecting django-filter==21.1 (from mercury)
  Downloading django_filter-21.1-py3-none-any.whl.metadata (5.1 kB)
Collecting markdown==3.3.6 (from mercury)
  Downloading Markdown-3.3.6-py3-none-any.whl.metadata (4.6 kB)
Collecting celery>=5.1.2 (from mercury)
  Downloading celery-5.4.0-py3-none-any.whl.metadata (21 kB)
Collecting sqlalchemy==1.4.27 (from mercury)
  Downloading SQLAlchemy-1.4.27.tar.gz (7.9 MB)
    ----- 7.9/7.9 MB 33.7 MB/s eta 0:00:00
Preparing metadata (setup.py) ... |
```

Installation will take some time. When the installation ends, it will look something like the below. Notice in the white text, the command prompt describes that it successfully installed several different packages.

(The red text is related to the **pip** package manager; we will not worry about this error.)

```
Microsoft Windows [Version 10.0.17134.470] (c) 2018 Microsoft Corporation. All rights reserved.

C:\Users\lrcguest> pip install random-walk-2d-mercury

Collecting random-walk-2d-mercury
  Using cached random-walk-2d-mercury-0.1.0-py3-none-any.whl
Installing collected packages: random-walk-2d-mercury
Successfully installed random-walk-2d-mercury-0.1.0

WARNING: The script mercury.exe is installed in 'C:\Users\lrcguest\AppData\Roaming\Python\Python311\Scripts' which is not on PATH.
Consider adding this directory to PATH or, if you prefer to suppress this warning, use --no-warn-script-location.

WARNING: The script mercury.exe is installed in 'C:\Users\lrcguest\AppData\Roaming\Python\Python311\Scripts' which is not on PATH.
Consider adding this directory to PATH or, if you prefer to suppress this warning, use --no-warn-script-location.

ERROR: pip's dependency resolver does not currently take into account all the packages that are installed. This behaviour is the source of the following dependency conflicts.
aioboto3 2.7.0 requires boto3<1.31.65,>=1.31.16, but you have boto3 1.29.165 which is incompatible.

Successfully installed amqp-5.2.0 asgiref-3.8.1 autobahn-23.6.2 billiard-4.2.0 bleach-6.1.0 boto3-1.26.83 botocore-1.29.165 celery-5.4.0 channels-4.1.0 click-didyoumean-0.3.1 click-plugins-1.1.1 click-repl-0.3.0 croniter-2.0.5 daphne-4.1.2 dj-rest-auth-3.0.0 django-4.2.7 django-allauth-0.52.0 django-cors-headers-3.10.1 django-drf-filepond-0.4.1 django-filter-21.1 django-storages-1.14.3 django-rest-framework-3.14.0 execnb-0.1.6 fastcore-1.5.45 gevent-24.2.1 ipywidgets-8.0.3 itables-2.1.1 kombu-5.3.7 markdown-3.3.6 mercury-2.4.2 oauthlib-3.2.2 pyee-8.2.2 pyppeteer-1.0.2 python3-openid-3.2.0 requests-oauthlib-2.0.0 s3transfer-0.6.2 shortuuid-1.0.13 sqlalchemy-1.4.27 sqlparse-0.5.0 txaio-23.1.1 urllib3-1.26.18 vine-5.1.0 websocket-client-1.8.0 websockets-10.4 whitenoise-6.6.0 widgetsnbextension-4.0.11 zope.event-5.0

(base) C:\Users\lrcguest>
```

Step 4: Find where mercury is installed

We need to find where **mercury** has been installed. Actually, our command prompt has given us some hints in the yellow **WARNING** text (depending on your environment, i.e., what has already been installed, you may or may not have this yellow text).

On the computer lab computers, mercury has been installed in the following path (note the use of the backslash, not the forward slash):

C:\Users\lrcguest\AppData\Roaming\Python\Python311\Scripts

Don't skip Step 5!

Step 5: Navigate to the folder where **random-walk-2d-mercury.ipynb** is using the change directory command (cd)

cd Downloads

Step 6: Run mercury

We are going to launch the mercury program through the command prompt. We will do this by entering the path to **mercury.exe**, followed by **mercury.exe**, and finally the command **run**. In this example, the command looks like the following.

```
C:\Users\lrcguest\AppData\Roaming\Python\Python311\Scripts\mercury.exe run
```

(Note: Ctrl+C/Ctrl+V copy/paste is possible in the command prompt). You should see something like the following appear in your command prompt session.



```

Anaconda Prompt - C:\Users\ww8844\AppData\Roaming\Python\Python311\Scripts\mercury.exe run
(base) C:\Users\ww8844\Downloads>C:\Users\ww8844\AppData\Roaming\Python\Python311\Scripts\mercury.exe run

mercury

Version: 2.4.2
Initialize random-walk-2D-mercury.ipynb
Successfully added a notebook (id:1)
Performing system checks...

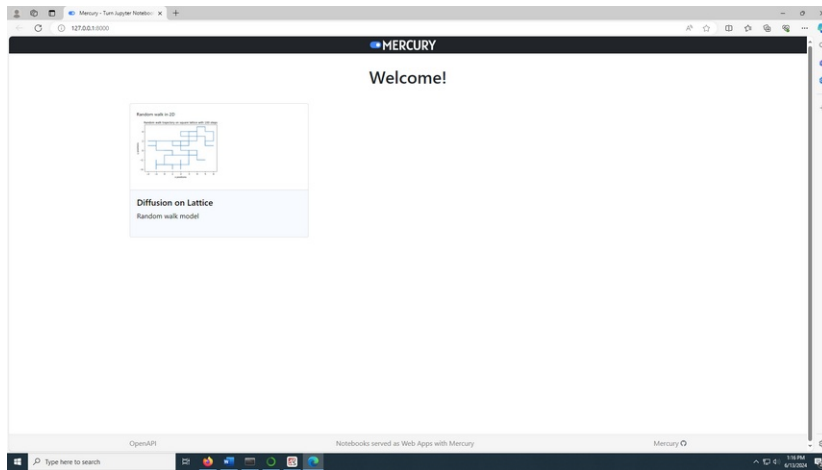
System check identified no issues (0 silenced).
June 13, 2024 - 13:14:19
Django version 4.2.7, using settings 'server.settings'
Starting ASGI/Daphne version 4.1.2 development server at http://127.0.0.1:8000
/
```

You might get a pop-up window that says something to effect of the task is something an administrator should run. Click “OK” to acknowledge.

Running mercury will launch new browser window that looks like the following

MITE 2024 Summer
Random Walk Diffusion Demonstration

Wang Materials Group
UT Austin



Click on the “Diffusion on Lattice” to bring you to the following page

