Setup Python, MLIP-Platform, and UMA Model (FAIRChem) on Windows using the PowerShell terminal in VSCode

Content

Install Python

You can install Python on Windows by following this tutorial:

https://www.digitalocean.com/community/tutorials/install-python-windows-10

(Note: Python3.11 recommended, FAIRChem currently supports Python <3.13, >=3.10 https://pypi.org/project/fairchem-core/)

Setup a Virtual Environment

A virtual environment isolates your Python packages for this project from other projects. The following steps are referenced from this tutorial:

https://packaging.python.org/en/latest/guides/installing-using-pip-and-virtual-environments/#create-and-use-virtual-environments

1. Create a virtual environment called ‘uma’.

In **PowerShell** within **VSCode**, navigate to a folder where you want your project (for example, E:\yifan\Projects\MLIP):

```
cd E:\yifan\Projects\MLIP
python -m venv uma
```

You will get the folder shown in the image:

2. Activate the virtual environment

.\uma\Scripts\activate

After running this, your PowerShell prompt should prepend with (uma) to indicate the venv is active.

```
PS C:\Users\12390> cd E:\yifan\projects\MLIP
PS E:\yifan\projects\MLIP> python --version
Python 3.11.0
PS E:\yifan\projects\MLIP> python -m venv uma
PS E:\yifan\projects\MLIP> .\uma\Scripts\activate
(uma) PS E:\yifan\projects\MLIP>
```

3. Install pip

pip is the reference Python package manager. It's used to install and update packages into a virtual environment.

You can make sure that pip is up to date by running:

python -m pip install --upgrade pip

```
(uma) PS E:\yifan\projects\MLIP> python -m pip install --upgrade pip
Requirement already satisfied: pip in e:\yifan\projects\mlip\uma\lib\site-packages (22.3)
Collecting pip
  Downloading pip-25.3-py3-none-any.whl (1.8 MB)
     ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 1.8/1.8 MB 5.4 MB/s eta 0:00:00
Installing collected packages: pip
  Attempting uninstall: pip
    Found existing installation: pip 22.3
    Uninstalling pip-22.3:
      Successfully uninstalled pip-22.3
Successfully installed pip-25.3
```

Verify pip is available by running:

python -m pip --version

```
(uma) PS E:\yifan\projects\MLIP> python -m pip --version
pip 25.3 from E:\yifan\projects\MLIP\uma\Lib\site-packages\pip (python 3.11)
```

Now your isolated environment is ready to install the required packages.

Setup MLIP-Platform

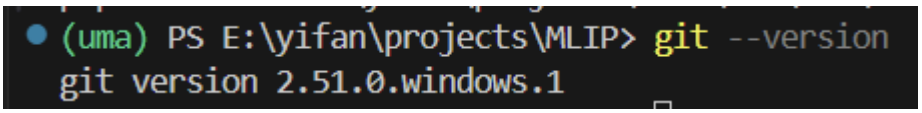
1. Install Git

1. Go to the official Git website: https://git-scm.com/downloads , Download the latest (2.51.2) x64 version of Git for Windows.
2. After the .exe file finishes downloading, double-click it to start installation.
3. During installation, you'll see several setup screens. The default settings are fine, but here are the key ones to check carefully:

Setup Screen	What to Choose	Why
Adjusting your PATH environment	✅ "Git from the command line and also from 3rd-party software"	Allows you to use `git` in PowerShell or VSCode terminal.
Choosing the default editor	You can keep "Vim" or select "VS Code" if you prefer.	VS Code is easier for most users.
Configuring line endings	"Checkout Windows-style, commit Unix-style line endings"	Recommended default for Windows.
Other options	You can leave everything as default.	Safe for most users.

4. Verify the installation: open the PowerShell terminal of VSCode and enter:

   git --version



2. Clone the MLIP-Platform repository

Before cloning and installing, don' t forget to activate venv:

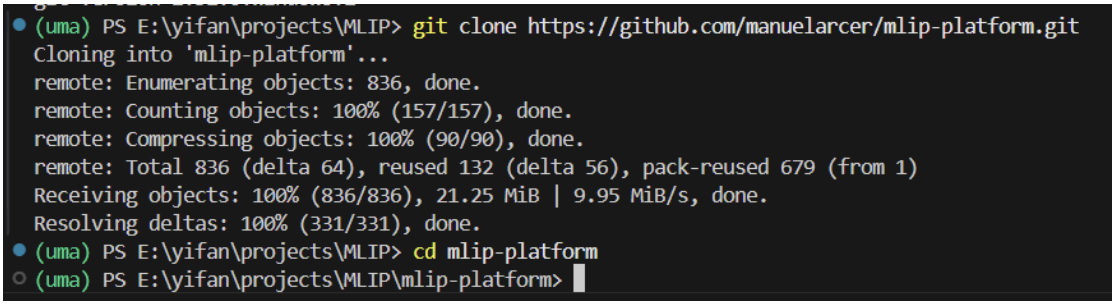
cd E:\yifan\Projects\MLIP

.\uma\Scripts\activate

Then Clone the repo:

git clone https://github.com/manuelarcer/mlip-platform.git

cd mlip-platform

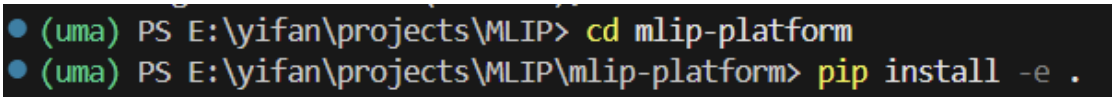


This downloads the code into a folder named mlip-platform and navigates into it.

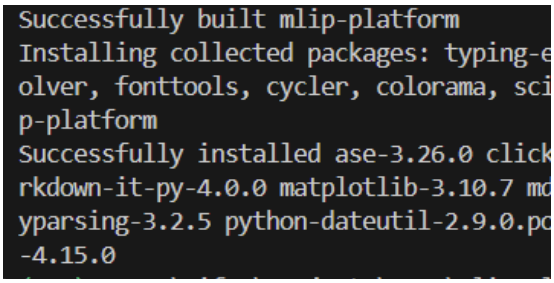
3. Install mlip-platform package

Still within the mlip-platform directory, run:

pip install -e .



The last few lines shown for successful installation:



The -e . option installs the package in editable (development) mode. This will set up the mlip command-line tool for you. After this, the mlip CLI should be available (as long as the ‘uma’ is active)

Setup UMA Model (FAIRChem)

Now we will install the FAIRChem-Core library from FAIR Chemistry team, which provides access to the UMA model and the ASE integration. The following steps are referenced from this tutorial: https://github.com/facebookresearch/fairchem?tab=readme-ov-file#fairchem-by-the-fair-chemistry-team

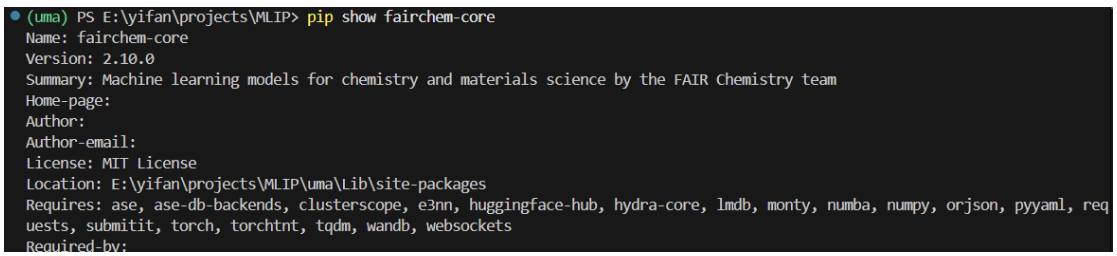
1. Install FAIRChem (fairchem-core)

From the PowerShell terminal (and ensure your venv 'uma' is activated), navigate out of the mlip-platform folder, back to your projects directory. Then run:

pip install fairchem-core

Verify the installation:

pip show fairchem-core



2. Login to Hugging Face for UMA Model Access

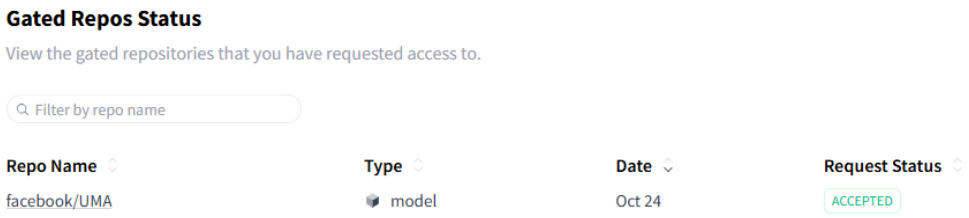
1. **Create a Hugging Face account:** If you don't have one, sign up for a free account. https://huggingface.co/join (Note: Please use your

work email address. Otherwise, your request for UMA model permission may be rejected.)

2. **Request access to the UMA model:** Log in to your Hugging Face account and navigate to the UMA model page. (https://huggingface.co/facebook/UMA) You will see a button to request access or agree to terms for the UMA model and apply for access.
3. **Check Access Status:**

   Go to your **profile icon → Settings → Gated Repositories**

   You will see the list as shown in the image:

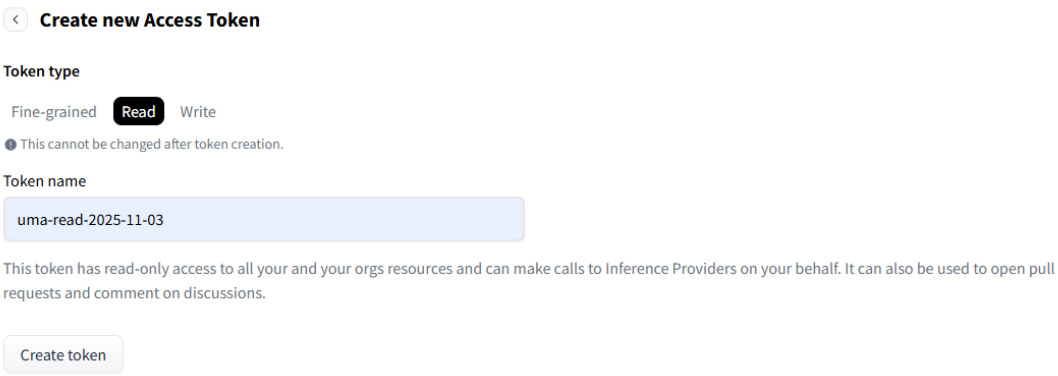


   "**ACCEPTED**" means you already have access.

4. **Generate an access token:**

   1) Go to your **profile icon → Settings → Access Tokens**

   2) Click "**New Token**", give it a name, and select the role as "**Read**" (read access to private models):



3) "**Create token**" and remember the generated token string, as it will not be seen anymore.

5. **Login to Hugging Face:**

Back in VS Code PowerShell (with the 'uma' active), If you did not install the Hugging Face hub tool, install it by running:

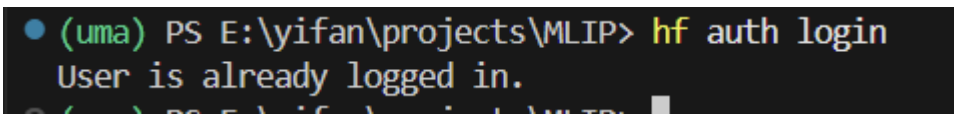
pip install huggingface_hub

After that run the login command:

hf auth login

When prompted, paste your token. This stores your token so Python libraries can use it to download the model.

After a successful login, your terminal will confirm you are logged in. (The token is saved in your user profile, so you typically only need to do this once.)



For more details, check out:

https://huggingface.co/docs/huggingface_hub/quick-start

Now your environment is set up! Start your work!