Polymer MD Workshop — Setup Guide

This guide provides step-by-step instructions to set up the environment for the **Polymer MD Workshop**.

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Quick Install

To quickly set up the environment, use the provided `setup_conda_env.sh` script.

Steps:

1. Download the GitHub repository containing the workshop scripts:

```
# Using wget
wget https://github.com/hargu978/polymermd-
workshop/archive/refs/heads/main.zip -O polymermd-workshop.zip
unzip polymermd-workshop.zip
cd polymermd-workshop-main

# OR using curl
curl -L https://github.com/hargu978/polymermd-
workshop/archive/refs/heads/main.zip -o polymermd-workshop.zip
unzip polymermd-workshop.zip
cd polymermd-workshop-main
```

2. Ensure the script has execute permissions:

```
chmod +x setup_conda_env.sh
```

3. If an old or incorrect environment with the name `polymer_md` exists, deactivate and delete it:

```
conda deactivate  # Deactivate the current environment (if any)
conda env remove -n polymer_md  # Delete the old environment
```

4. Run the script:

```
./setup_conda_env.sh
```

This script will:

- Check if Conda is installed, and install Miniconda if necessary.
- Create the Conda environment using the `environment.yml` file.
- Activate the environment and source AmberTools.

> **Note:** Ensure the `setup_conda_env.sh` script and `environment.yml` file are in the same directory.

Step 1: Install Conda

For Linux or macOS:

1. Download the Miniconda installer:

```
# For Linux
wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh

# For macOS
curl -O https://repo.anaconda.com/miniconda/Miniconda3-latest-MacOSX-x86_64.sh
```

> **Estimated time:** ~1-3 minutes (depending on network speed)
> **Minimum disk space:** ~100 MB for the installer

2. Run the installer:

```
bash Miniconda3-latest-<OS>-x86_64.sh  # Replace <OS> with Linux or MacOSX
```

> **Estimated time:** ~2-5 minutes
> **Minimum disk space:** ~400 MB for installation

3. Follow the prompts to complete the installation.

4. Delete the installer file:

```
rm Miniconda3-latest-<OS>-x86_64.sh
```

> **Estimated time:** ~1 second

5. Activate Conda:

```
source ~/.bashrc
```

> **Estimated time:** ~1 second

Step 2: Create the Conda Environment

1. Ensure the `environment.yml` file is in the project root directory:

```
name: polymer_md
channels:
  - conda-forge
  - dacase
dependencies:
  - python=3.12
  - ambertools-dac=25     # AmberTools (Linux/macOS via dacase)
  - gromacs
  - parmed
  - openbabel
  - pip
  - pip:
      - nglview
      - jupyter
```

2. Create the environment:

```
conda env create -f environment.yml
```

> **Estimated time:** ~2-10 minutes (depending on the environment complexity)
> **Minimum disk space:** ~1 GB (depending on the packages in `environment.yml`)

3. Activate the environment:

```
conda activate polymer_md
```

> **Estimated time:** ~1 second

4. Source the AmberClassic environment:

```
source $CONDA_PREFIX/AmberClassic.sh
```

> **Estimated time:** ~1 second
> **Minimum disk space:** AmberClassic installation size (if not already installed)

Step 3: Start Jupyter Lab

1. Verify the installation of core tools:

```
gmx --version           # GROMACS
antechamber -h          # AmberClassic / Antechamber
parmchk2 -h             # Parmchk2
tleap -h                # tleap (Amber)
obabel -V               # Open Babel
jupyter --version       # Jupyter
```

> **Estimated time:** ~1-2 minutes (to verify all tools)

2. Start Jupyter Lab:

```
jupyter lab --ip 0.0.0.0 --no-browser
```

> **Estimated time:** ~5-10 seconds

3. Open the URL printed in the terminal to access Jupyter Lab.

Notes

- If any tool is missing, install it manually:

```
conda install -c conda-forge gromacs parmed openbabel
conda install dacase::ambertools-dac=25
pip install nglview jupyter matplotlib
```

> **Estimated time:** ~2-5 minutes (depending on the missing tools)
> **Minimum disk space:** ~500 MB - 1 GB (depending on the tools)

- Refer to the following for more information:
  - Jupyter Notebook Basics
  - Jupyter Lab Interface

Day 1: Notebook & Example Commands

Purpose

Demonstrate a compact AmberTools workflow:

1. Convert SMILES → 3D PDB (OpenBabel)
2. Run antechamber to assign GAFF atom types & AM1-BCC charges
3. Run parmchk2 to generate missing force-field terms (.frcmod)
4. Use tleap to create prmtop and inpcrd files

Example Commands

```
# 1. SMILES -> 3D PDB (OpenBabel)
obabel -:"CCO" -O ethanol.pdb --gen3d
# Estimated time: ~5 seconds

# 2. Antechamber: generate mol2 and AM1-BCC charges
antechamber -i ethanol.pdb -fi pdb -o ethanol.mol2 -fo mol2 -c bcc -s 2
# Estimated time: ~10-30 seconds

# 3. Parmchk2: create frcmod
parmchk2 -i ethanol.mol2 -f mol2 -o ethanol.frcmod
# Estimated time: ~5 seconds

# 4. tleap: build prmtop/inpcrd
cat > tleap_ethanol.in << 'EOF'
source leaprc.gaff
ETH = loadmol2 ethanol.mol2
loadamberparams ethanol.frcmod
saveamberparm ETH ethanol.prmtop ethanol.inpcrd
quit
EOF

tleap -f tleap_ethanol.in
# Estimated time: ~5-10 seconds
```

The Day-1 notebook contains these steps with explanatory text and cells you can run interactively.