Installation

Environment Setup

Using Conda

- Download `MPicker_code.tar.gz`.
- Uncompress it into an empty folder. Let's call it `/absolute/path_to/save_code`. Replace it with the actual path where you want to install MPicker.

  ```
  mkdir /absolute/path_to/save_code
  tar -zxvf MPicker_code.tar.gz -C /absolute/path_to/save_code
  ```

- You can edit the `env.yml` file in the folder `path_to/save_code/mpicker_gui`:
  - Change "mpicker_full" to your preferred environment name.
  - Modify "`cudatoolkit=11.0`" to another version if your GPU driver doesn't support it (e.g., =10.1 or =9.2).
  - The library versions don't have to match exactly as in the yml file. We just provide the versions we use. However, `scipy>=1.7`, `yacs>=0.1.8`, and `pyqt=5` must be satisfied. We choose `open3d=0.9.0` for compatibility with older systems, but newer versions are allowed if your machine supports it.
- Create the Conda environment from this file (may take 10 minutes or more):

  ```
  conda env create -f path_to/save_code/mpicker_gui/env.yml
  ```

- Finally, activate the environment with:

  ```
  conda activate mpicker_full
  ```

Without Conda

We still recommend using Conda because our offline environment package is quite large, and Conda is commonly used in Python. You can install Conda from https://docs.conda.io/projects/miniconda/en/latest/.

We generate the environment packages using conda-pack on CentOS7, but it should work for other Linux systems. You have to use Conda if your system is not Linux.

- Download `MPicker_environment.tar.gz` and `MPicker_code.tar.gz`.
- Uncompress them into two **different** empty folders. Let's call them `/absolute/path_to/save_code` and `/absolute/path_to/save_env`. Replace them with the real paths where you want to install MPicker.

  ```
  mkdir /absolute/path_to/save_code
  tar -zxvf MPicker_code.tar.gz -C /absolute/path_to/save_code
  mkdir /absolute/path_to/save_env
  tar -zxvf MPicker_environment.tar.gz -C /absolute/path_to/save_env
  ```

- Unpack the Conda environment (only need to do this once):

  ```
  source path_to/save_env/bin/activate
  conda-unpack
  source path_to/save_env/bin/deactivate
  ```

After installation, you can activate the environment using:

```
source path_to/save_env/bin/activate
```

and deactivate it using:

```
source path_to/save_env/bin/deactivate
```

Environment Setup without Membrane Segmentation

This version doesn't include AI-based automatic membrane segmentation but requires less libraries and has a smaller installation size.

- Replace `MPicker_code.tar.gz` with `MPicker_code_noseg.tar.gz`, which lacks the folder `memseg_v3`.
- Replace `MPicker_environment.tar.gz` with `MPicker_environment_noseg.tar.gz` if you set up environment without Conda.
- Replace the `env.yml` file with `env_simple.yml` if you set up environment by Conda.
- In fact, you can use most of MPicker's functions in the environment of IsoNet, but `scipy` must be >=1.7.

Get Started

Quick Start Guide

First, activate the environment. Verify the Python environment using:

```
which python
```

Expect a path like:

```
path_to/save_env/bin/python # if without conda
path_to/miniconda/envs/mpicker_full/bin/python # if using conda
```

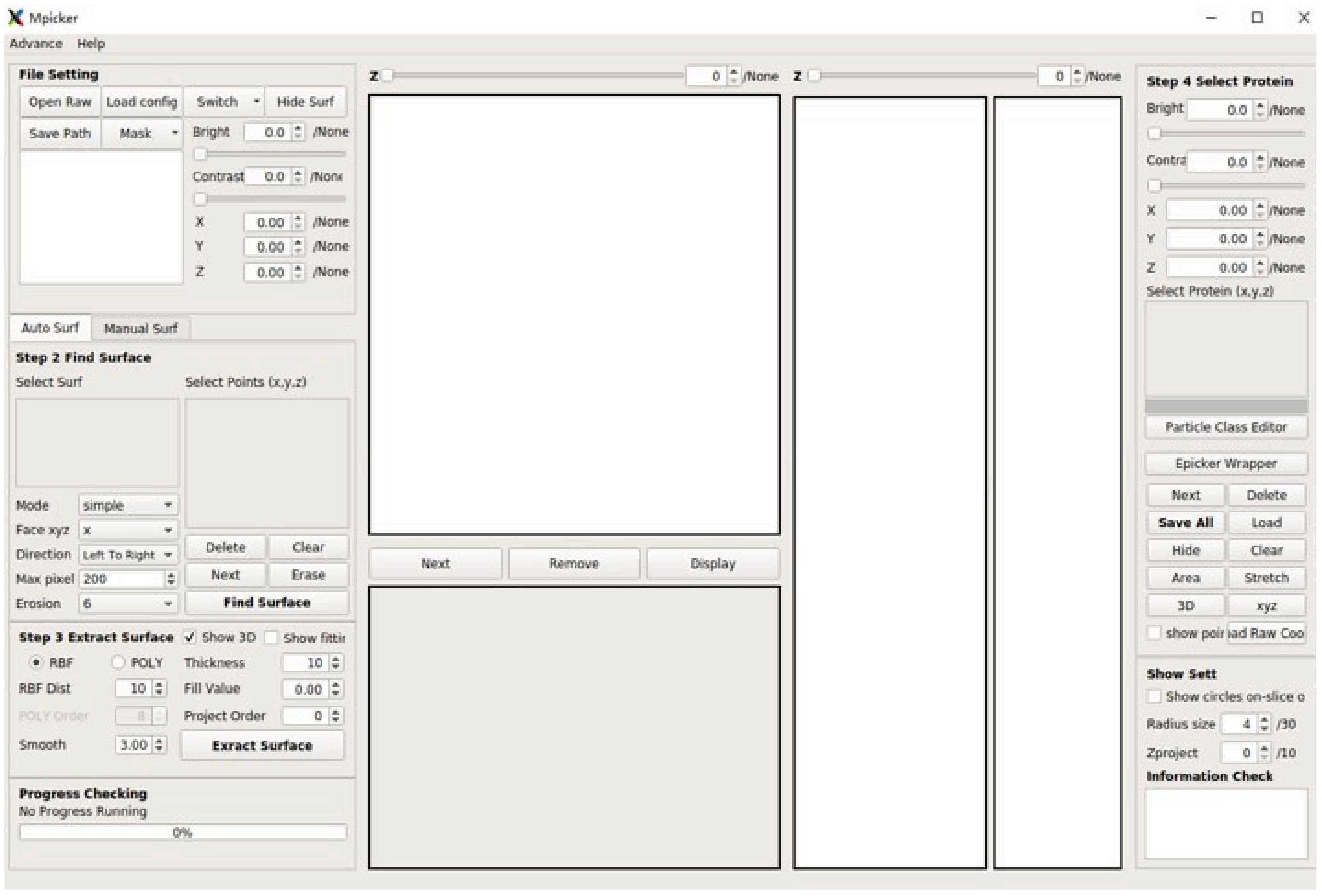
Run the following command to open Mpicker:

```
python path_to/save_code/mpicker_gui/Mpicker_gui.py
```

Alternatively, add `path_to/save_code/mpicker_gui` to your `$PATH` and open Mpicker with:

```
Mpicker_gui.py
```

Then you will get the following GUI:



Troubleshooting

- For Linux users: If your shell is not bash (e.g., csh), switching to bash may resolve environment setup issues. Check your shell using:

```
echo $0
```

- If executing .py files directly fails, try running `bin/mpicker.sh`, a bash wrapper. Add `path_to/save_code/bin` to your PATH, activate the environment, and run MPicker using:

  ```
  mpicker.sh
  ```

- Modify `PYTHON="$(which python)"` in `bin/mpicker.sh` to `PYTHON=/absolute/path_of/python` if your system fails to locate the installed Python. This allows running Mpicker with `mpicker.sh` without activating the environment first.

Command Start

Mpicker support these parameters input from command line:

`--raw Path of raw tomogram map`

`--mask Path fo mask tomogram map`

`--out Existed path to save all the result files`

`--config Path of config file (config file for reloading all the process history)`

Example: (Open a new GUI)

```
Mpicker_gui.py --raw tomogram.mrc --mask segmentation.mrc --out ./
```

Example: (Reload a existing job)

```
Mpicker_gui.py --config ./tomogram.config
```