Manual

1 Installation

MD2D needs the dependencies:

numpy

scipy

matplotlib

mdanalysis

It can be installed locally. Under the package directory.

```
> pip install   .
```

Besides, MD2D and its required dependencies can be installed using pip:

```
> pip install md2d
```

2 Files

Input:

MD2D reads the output of molecular dynamics simulations in the VASP format. Only two input files will be read: XDATCAR and OUTCAR.

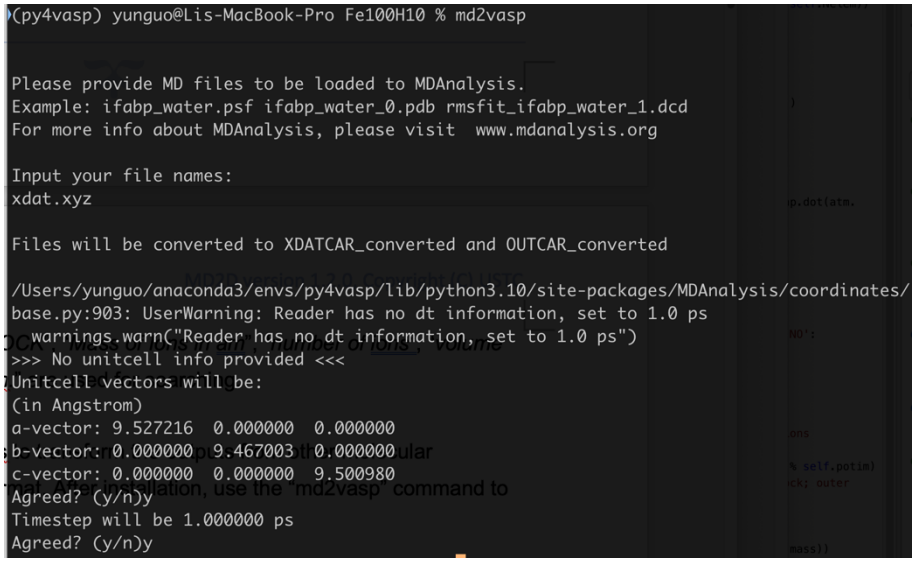
XDATCAR: MD2D reads in the trajectory from XDATCAR.

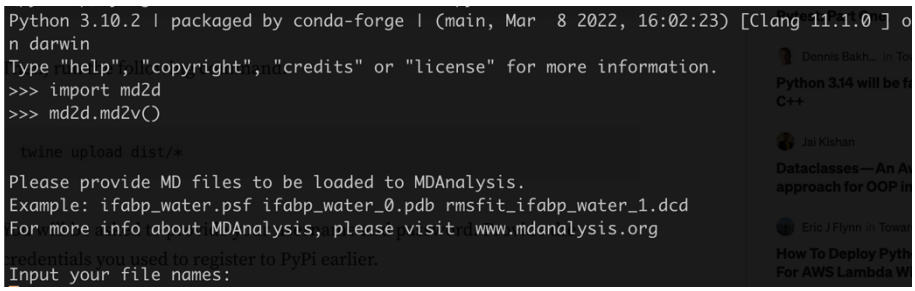
OUTCAR: MD2D reads in the following lines from OUTCAR:

- *POTIM = 1.0000   time-step for ionic-motion*
- *NBLOCK =   1;   KBLOCK =   1   inner block; outer block*
- *Mass of Ions in am*
  POMASS = 55.85
- *volume of cell :   711.71*
- *kin. lattice EKIN_LAT=   93.098925 (temperature 7275.16 K)*
- *Total+kin.   3416.08 3605.40 3585.13   -42.72 -109.39   -38.68*

The keys words “*POTIM*”, “*NBLOCK*”, “*Mass of Ions in am*”, “*number of ions*“, “*volume of cell*”, “*EKIN_LAT=*”, “*Total+kin.*” are used for searching.

Besides, MD2D uses MDAnalysis to transform the outputs from other molecular dynamics codes to the VASP format. After installation, use the “md2vasp” command to initiate the conversion, or call the “md2v” function.





Output:

Calculated diffusion coefficients, viscosities, and correction to diffusion coefficient are streamed in standard output. Besides, D-τ, mean squared displacement (MSD) and stress auto-correlation function (SACF) will be written into file as X_D_tau.dat (X is the element name), msd.dat and sacf_average.dat, and their plotsare saved as D_tau.pdf, msd.pdf and SACF.pdf. In each X_D_tau.dat, the first column is the time interval, the left three columns are the Ds for x, y and z directions. The columns in msd.dat

corresponds to the MSDs for the elements in the order provided in XDATCAR. The three columns in sacf_average.dat are the MD step, bulk SACF and shear SACF.

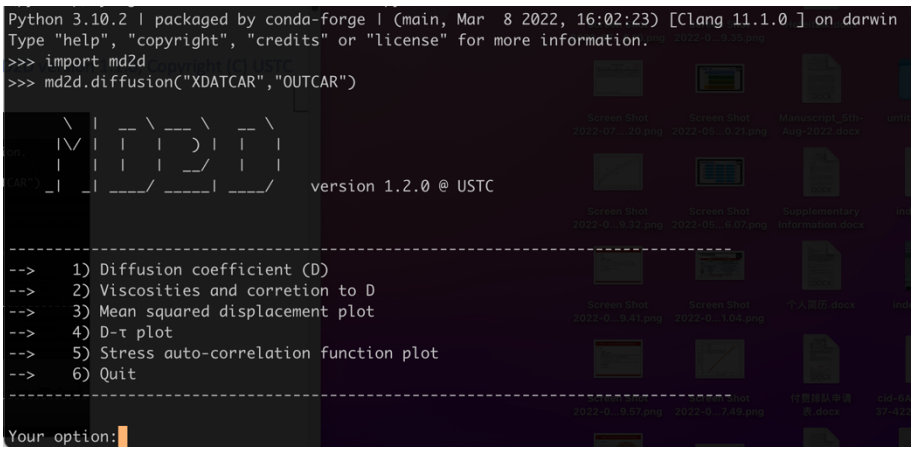
3 How-To Guides

3.1 Launch the code

Simply import the package within python, and enter the menu by typing:

```
> import md2d
> md2d.diffusion(xdatcar="XDATCAR", outcar="OUTCAR")
```

It takes two variables: the names of input files. Default values will be XDATCAR and OUTCAR.

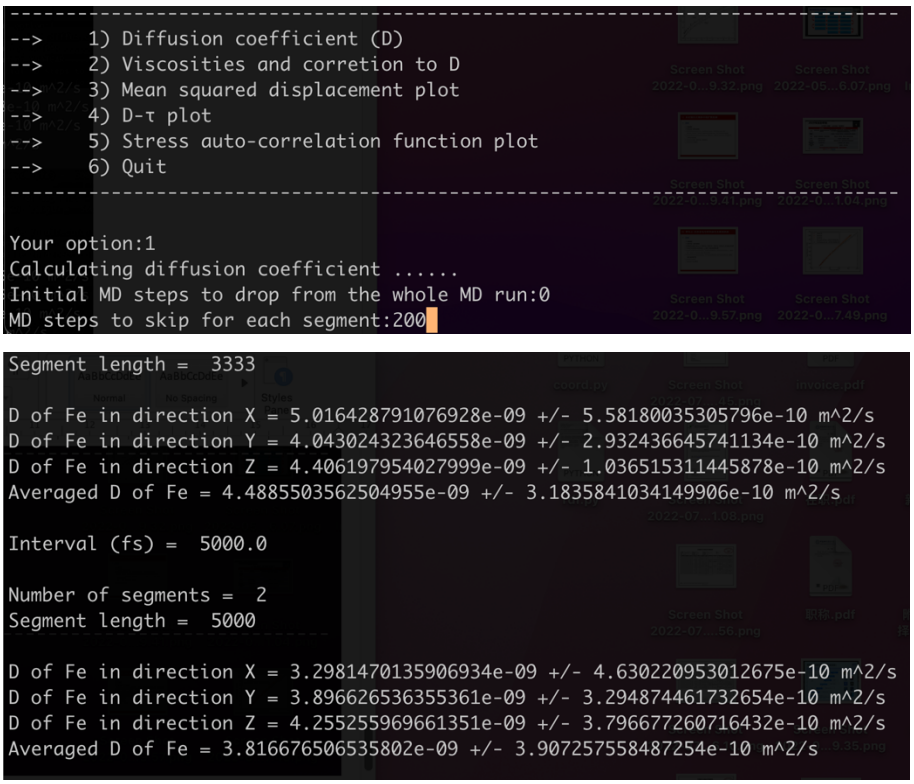


3.2 Calculate diffusion coefficient

Choose option 1 will lead to the calculation of diffusion coefficient. Then, MD2D will exhaust the available time intervals to calculate the diffusion coefficient as a function of time interval. The procedure and results will be streamed on the screen, and the D-τ data will be written into the file X_D_tau.dat.

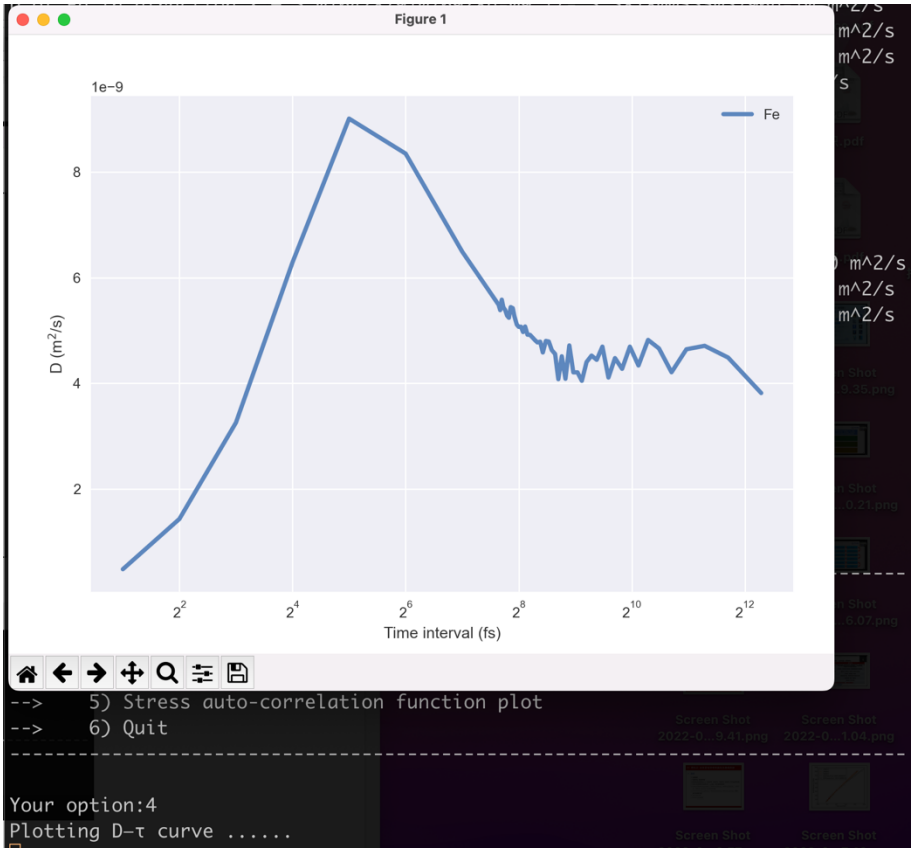
Two integer parameters will be asked for, namely, the number of initial MD steps to drop and the number of MD steps to skip for each segment. The first is to drop out the unwanted/unequilibrated initial stage of MD. The second is to exclude the ballistic

motion stage from fitting the Einstein relation. The second parameter can be determined from the log-log plot or MSD.

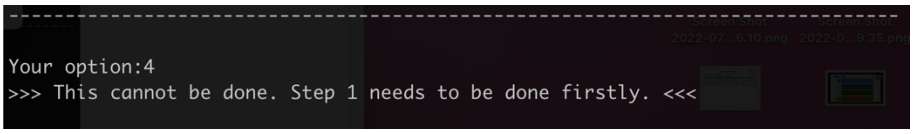


3.3 Plot D-τ

If diffusion coefficients have been calculated by doing option 1, then choose the option 4 will plot the D-τ curve.

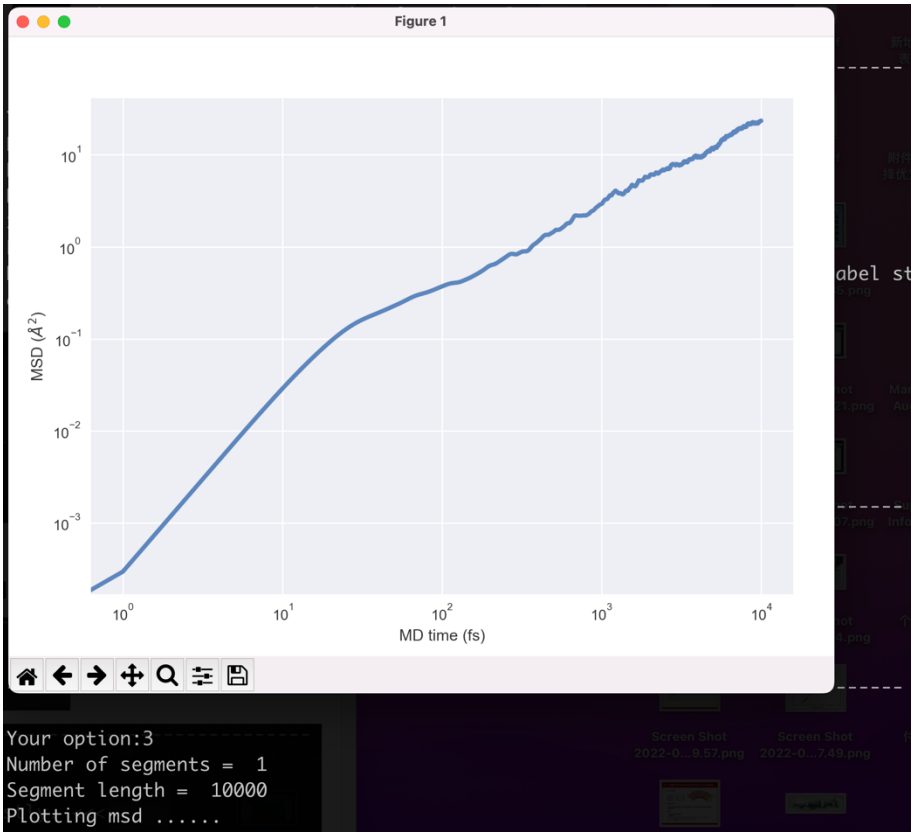


If step one hasn't been done, they a warning message will prompt to do option 1 firstly.



3.4 Calculate MSD

The MSD can be calculated and plotted by choosing option 3. The plot usually sees a change of trending, and the length of the first part is the length of ballistic motion that needs to be removed from fitting the Einstein relation.



3.5 Calculate viscosities and correction to diffusion coefficient

The stress auto-correlation function, viscosities, and correction to diffusion coefficient will be calculated by choosing option 2. The results will be streamed on the screen. The correction to diffusion coefficient is best applied to single-component system, e.g., pure Fe liquid or molecular liquid. For complex system like silicate melt, an element- or component-wise correction according to Eq. (4) in Li and Ni, (2022) should be considered.

```
Your option:2
Calculating viscosities ......
Reading stresses from OUTCAR ......
Calculating stress auto-correlation function ......
Calculating viscosity from stress auto-correlation function ......
Calculated bulk and shear viscosities are:
0.0046357311181300966, 0.012556958898286735  (Pascal*Second)
Their uncertainties are:
0.002400124549182609, 0.0011427835182706988  (Pascal*Second)

Calculated correction to D is:
1.6695706485186846e-09 +/- 1.4037282864630724e-10  (m^2/s)

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     |\/ |  |   |   ) |  |   |
     |   |  |   |  __/   |   |
    _|  _| ____/ _____| ____/    version 1.2.0 @ USTC
```
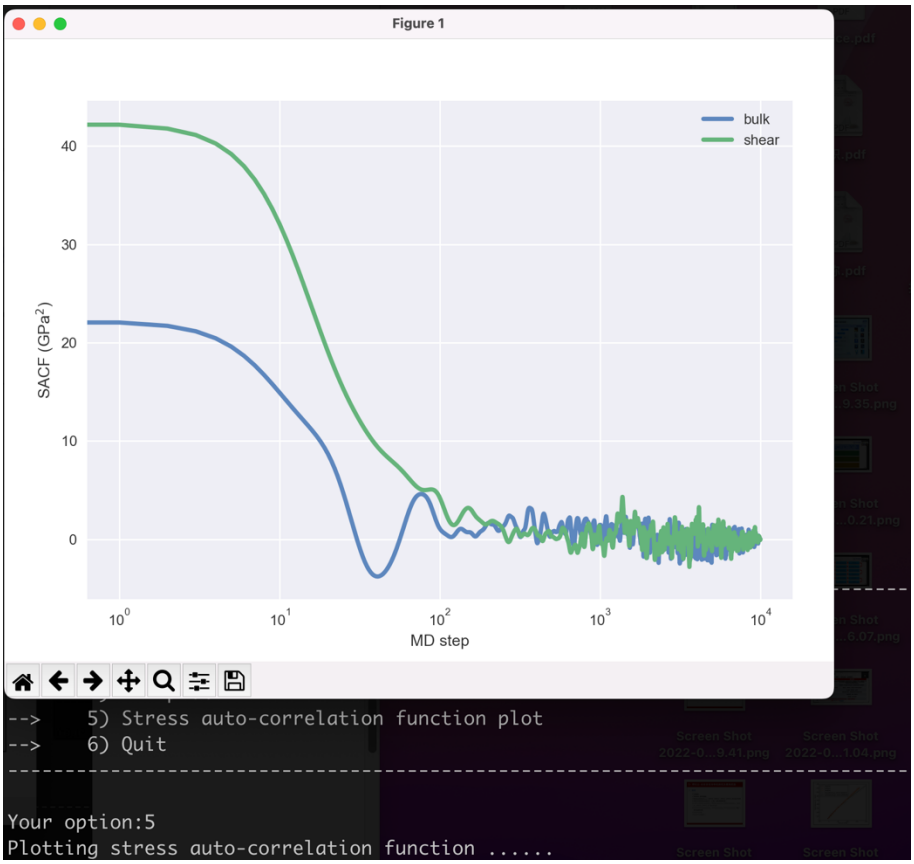
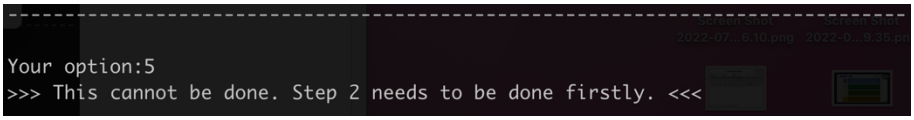

3.6 Plot stress auto-correlation function

The stress auto-correlation function can be plotted by choosing option 5 after finishing the calculation in option 2. Otherwise, MD2D will ask for doing option 2 firstly.





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