Tutorial

Last update: 20th November 2023
Reference version of MIPET 1.0.0.0\

Contents

Introduction

MIPET (Mesoscopic Interaction Parameter Estimation with Tinker) is an automated pipeline for comprehensive calculation of intermolecular interaction energies and coordination numbers based on molecular force-fields using the Tinker molecular modeling package. A scientific article describing MIPET can be found here . The MIPET GitHub repository were you can download the software, browse the source code, and report issues can be found here.

Installation and start-up

Pre-compiled and executable MIPET distributions can be found attached to the marked releases. Please note that MIPET only supports x64 architecture in general.
With this tutorial and on the first run after a fresh installation a short "proof-of-work" calculation is configured. It should take about 10 to 15 min. The tutorial files can be found in the Tutorial folder of MIPET and must be copied to the appropriate places to repeat the tutorial calculation.

Windows

A convenient dedicated Windows OS installer executable for MIPET is available here , it comprises a full Java runtime environment. Download the installer executable, start, and follow the instructions to install the calculation pipeline. Follow the instructions for the Tinker installation. To run the pipeline, a scratch directory must be configured in the MIPET.properties file, which can be found in the "resources" directory. Then simply double-click on the batch file "MIPET.bat".

Should this installation or the execution of the batch files not work for you, try the guidelines for Linux described below. As an alternative way, they should also work on Windows.

Linux

Every release has a zip file attached which contains the MIPET Java archive with all dependencies (except Tinker) and a full Java runtime environment (click here to automatically download the zip file of the latest version). After extracting the zip file, follow the instructions for the Tinker installation. To run the pipeline, a scratch directory must be configured in the "MIPET.properties" file, which can be found in the "resources" directory. Then execute the JAR from the command line.

Tinker

In order to run MIPET, the Tinker molecular modeling tool package has to be added. For this, the Tinker executables and the files for the atomic parameters of version 8.10.2 have to be downloaded (click here to go to the Tinker website). Choose the correct version for your OS. Please note the current licence. The executables and the parameter files have to be placed in a subfolder named "tinker", which you have to create in the root directory of MIPET. Exampled directory structure:

```
├── MIPET                  # MIPET root directory
│   ├── ...
│   ├── tinker             # Frequently asked questions
│   │  ├── params          # Directory to put parameter files
│   │  ├── alchemy.exe     # Tinker executable
│   │  ├── analyze.exe     # Tinker executable
│   │  └── ...             # more Tinker executables
│   └── ...
```

Change calculation properties, molecules and force fields

The "MIPET.properties" file, which can be found in the "resources" directory, allows to change properties for a calculation. For example, to adjust the number of evenly spaced points on the spheres for the calculation of the intermolecular energy, the "MIPETSphereNodeNumber" setting can be changed. Each property in this file has a short comment describing what it does. To change the used molecules the file "MIPET.job" holds a section named "Particles". The molecules to use must be listed in this section by using their abbreviations. To not consider a molecule during the pipeline a preceded hashtag is needed. Configured and ready-to-use molecules can be found in the "Molecules" folder, seperated by different force fields. To create and configure new molecules for the calculation pipeline follow the instruction of the section Create and configure molecules.
Different force fields can be used to calculate the intermolecular energy and determine the coordination number. The force field to be used for calculating the intermolecular energy must be preceded by an asterisk and the force field to be used for calculating the coordination number must be preceded by a dollar sign.

Configure water model

To configure the water model for the force fields OPLSAA and SMOOTHAA just copy and paste the file of the chosen water model inside the force field directory and rename the new file to "H2O.xyz". By default, after a fresh installation, and if nothing was changed, the TIP5P water model is chosen.

Create and configure molecules

To create a new molecule file in the Tinker xyz file format, which can be used in the calculation pipeline, a mol file of the desired molecule is needed. This mol file can be transformed into a Tinker xyz file by using the Tinker tool "mol2xyz". Therefore, a key file is needed which refers to the parameter file of the desired force field, e.g. for OPLSAA:

```
PARAMETERS "<Path to Tinker directory>\Tinker\params\oplsaa.prm"
```

The Tinker xyz file generated for methanol using this method looks like the following:

```
6    MeOH
1  C      0.680000   -0.025000    0.000000     0     2     3     4     5
2  H      1.047000    1.011000   -0.000000     0     1
3  H      1.009000   -0.547000   -0.904000     0     1
4  H      1.009000   -0.547000    0.904000     0     1
5  O     -0.746000    0.124000    0.000000     0     1     6
6  H     -1.172000   -0.756000    0.000000     0     5
```

The first row following the coordinates must be replaced with the corresponding atom type numbers of the force field:

```
6    MeOH
1  C      0.680000   -0.025000    0.000000     99     2     3     4     5
2  H      1.047000    1.011000   -0.000000     98     1
3  H      1.009000   -0.547000   -0.904000     98     1
4  H      1.009000   -0.547000    0.904000     98     1
5  O     -0.746000    0.124000    0.000000     96     1     6
6  H     -1.172000   -0.756000    0.000000     97     5
```

This file must be copied in the directory of the force field inside the "Molecules" directory.