Manual

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This is the documentation of a *python* class for generating polymer simulations LAMMPS scripts.

The simulations two kind of systems are generated by this class. One is the simulation of polymer chains diffusing in a matrix of moving spheres, and the other kind is the simulation of polymer chains diffusing in empty space.

This class can be accesed and downloaded in this link.

CHAPTER

ONE

USER DOCUMENTATION

1.1 Getting started

1.1.1 Installing NumPy

To be able to use this class, first one must have NumPy library installed, which is of keen importance to this class. If you are using Anaconda, you are safe to proceed. If not, this library can be installed by doing on you're bash:

```
pip3 install numpy
```

1.1.2 Installing fortran

This class is a result of a python and a fortran joint code. To proceed, we need to install gfortran to be able to fully execute this class. To install gfortran on Linux systems, execute the bellow command on you're bash:

```
sudo apt-get install gfortran
```

1.1.3 Installing LAMMPS

Since this class generates LAMMPS scripts for polymer simulations, you must have LAMMPS installed on you're workstation. To do this, please, access this link.

1.2 Class description

class lammps_generator.**PolymerSimulation**(*system_parameters*, *pathto*)

This is the class PolymerSimulation. After specifing the needed system parameters, it will execute the chain.f, or chain_alone.f, code for the polymers input generation, and then it will write the LAMMPS inputs for running. chain.f is for the case of mixing polymers with obstacles, and the chain_alone.f is for when one wants only to simulate polymers in empty space.

Parameters

- **system_parameters** – A dictionary with important system parameters.
- **pathto** – A path to the class directory location.

1.3 System parameters

1.4 Output code

CHAPTER

TWO

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