Guidelines for Generating Trajectories for Data in "Simulating precursor steps for fibril formation in methylcellulose solutions", Phys. Rev. Materials **3**, 055601 (2019)

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May 16, 2019

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1 Required Software Packages and Compilers

This document deals with the codes used in this work, software required, code dependencies (wherever applicable), and instructions to generate initial configuration.[1]

1. LAMMPS package - Version: Aug-17-2017 or later with MPI compatibility.
2. Fortran 90/95 with ifort, mkl and openmp compilers.
3. MATLAB 2017b or later.
4. Python 3.0 or later.

2 LAMMPS codes

1. in.cgpair_MC - contains interaction parameters.
2. in.cgrun1 - initial equilibration code.
3. in.cgrun2, in.cgrun3 - multiple rounds of equilibration code.
4. in.cgrun4, in.cgrun5 - production codes with different time steps.

3 FORTRAN codes

1. ran_numbers.f90 - code to generate random numbers based on present computer time.
2. lammps_inp.f90 - code to generate chains with random initial configuration for using with LAMMPS.
3. lmp_params.f90 - code containing parameters for generating different structures.
4. lmp_params_var.f90 - replicate of lmp_params.f90, but for usage with Python codes for parameter sweeps.
5. replicate_diff_geometry.f90 - code to replicate a structure given the eigenvalues of gyration tensor for usage with LAMMPS.
6. create_infile.f90 - code to generate interaction parameters depending upon temperature.
7. infile_params.f90 - parametric file for create_infile.f90
8. main.f90 - main analysis code.
9. params.f90 - parametric file for main.f90
10. inprep.txt - sample input file containing details of rings and required final configuration for replicating.
11. anainp.txt - sample input file containing details of the analyses required.

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4 MATLAB Codes

1. plot_generic_kappa.m - generates color bar data for shape anisotropy factors (see Fig. 8 in main paper).
2. consolidate_eigendata.m - consolidates eigenvalues to use with plot_generic_kappa.m.
3. analyze_kappa.m - computes eigenvalues and shape anisotropy factors.
4. pl_indkap.m - plots shape anisotropy factor (for each chain) as a function of time for one system (required dependency for plot_generic_kappa.m – keep in the same folder).
5. pl_indeig.m - plots individual eigenfactors as a function of time for one system (required dependency for plot_generic_kappa.m – keep in the same folder).
6. read_analyze_indeig.m - required dependency for consolidate_eigendata.m (keep in the same folder)
7. genplane.m - computes eigenvalues and eigenvectors after fitting a plane to a single ring to use with replicate_diff_geometry.f90.

5 Python Codes

1. genconf.py - To generate configurations using different FORTRAN files.
2. ana.py - To analyze configurations using main.f90 and params.f90.

6 Running FORTRAN Codes

- To generate single chain initial configuration:
  `ifort -r8 -qopenmp -mkl ran_numbers.f90 lmp_params.f90 lammps_inp.f90`
- To replicate geometry:
  `ifort -r8 -qopenmp -mkl ran_numbers.f90 replicate_diff_geometry.f90 -o rep.out; .\rep.out inprep.txt`
- To analyze trajectories:
  `ifort -r8 -qopenmp -mkl params.f90 main.f90 -o ana.out; .\ana.out anainp.txt`

7 Running LAMMPS codes

To generate the trajectories, run `in.cgrun?` in succession using LAMMPS executable file. Make sure the supporting files like `in.cgpair_MC` and input data file (see respective in.cgrun1 to see the name of the data file used) are in the same folder. While compiling LAMMPS the `MOLECULE` package should be added.