Research data supporting 'Microscopic analysis of thermo-orientation in systems of off-centre Lennard-Jones particles'

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This document is part of the supporting data for

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The procedure to obtain the simulation data reported in the paper is as follows:

– The data repository (doi:10.17863/cam.37306) includes a modified version of LAMMPS (11Aug17) that includes the following additional source files:

  – `pair_lj_cut_alpha_site.h/cpp`,
  – `fix_gauss_local.h/cpp`.

The `.cpp` files contain further documentation about these modifications. To prepare this modified version of LAMMPS for execution:

1. Download the file `lammps-11Aug17_mod.tbz2` and make sure that it is located in your current directory.
2. Unpack the file `lammps-11Aug17_mod.tbz2` and change to the directory `src`.
   ```
   $ tar xjf lammps-11Aug17_mod.tbz2 && cd lammps-11Aug17_mod/src
   ```
3. Compile LAMMPS for parallel execution. To do this, you may wish to modify the file `MAKE/Makefile.mpi` to select your preferred compiler (the default compiler is `mpiicc`).
   ```
   $ make -j4 mpi
   ```
   After successful execution of this command, the current directory should contain an executable file called `lmp_mpi`.

– Download the `simulations-and-analysis.tar.bz2` file, extract it, and run LAMMPS with the input script provided (`simulation/nemd.lammps`).

– This will produce the file `correlations.dat`. This file lists a number of properties for each of the 20 bins that the box is partitioned into along the z axis. One line is provided for each bin, and the same sequence is repeated every 50 steps (following an appropriate header). The columns in the data lines correspond to the following properties, averaged over all particles in a given bin:

(1) bin number

(2) z co-ordinate of bin

(3) $|\boldsymbol{p}|^2/(md)$ (local temperature)

(4) ρ

(5) f_z

(6) e_z

(7) $L^2/2I$

(8) $p^2/2m$

(9) $e_z L^2/2I$

(10) $e_z p^2/2m$

(11) $\boldsymbol{e}\cdot\boldsymbol{f}$

(12) $e_z(\boldsymbol{e}\cdot\boldsymbol{f})$

(13) $\alpha f_z - e_z(\boldsymbol{e}\cdot\boldsymbol{f})$

(14) $(\boldsymbol{L}\times\boldsymbol{e})\cdot\boldsymbol{p}$

(15) $e_z(\boldsymbol{L}\times\boldsymbol{e})\cdot\boldsymbol{p}$

(16) $(\boldsymbol{L}\times\boldsymbol{e})_z(\boldsymbol{f}\cdot\boldsymbol{L}\times\boldsymbol{e})$

(17) $(\boldsymbol{L}\times\boldsymbol{e})_z(\boldsymbol{f}\cdot\boldsymbol{p})$

(18) $p_z((\boldsymbol{L}\times\boldsymbol{e})\cdot\boldsymbol{f})$

(19) $p_z(\boldsymbol{f}\cdot\boldsymbol{p})$

(20) $(\boldsymbol{L}\times\boldsymbol{p})_z$

– These data should then be averaged over time and the results analysed with the script provided (`analysis/proc_v3.py`). This script expects input files to be provided using the same columns as above, except that every column bar the bin number should be followed by the standard deviation of the measurement. A full description of the expected columns is provided in the comment at the start of the script. The script is written in Python 2.7.

Several files with averaged data are provided in the directory `analysis` and can be analysed with the `proc_v3.py` script. These files are named `T`T`_Rho`ρ`_alpha`α`_correlations.avg`, where T, ρ and α correspond to the (average) temperature, number density and the centre-of-mass–LJ shift used. We also provide three files with analysed data that were used to plot the figures in the manuscript: `analysed-alpha.dat`, `analysed-T1.dat` and `analysed-T125.dat`.

These files can be obtained using the command

```
$ python2.7 proc_v3.py | awk '/#summary / { $1=""; print > "analysed-alpha.dat";} \
                              /#T1 / { $1=""; print > "analysed-T1.dat";} \
                              /#T125 / { $1=""; print > "analysed-T125.dat"; }'
```

The columns in the `analysed-alpha.dat` file correspond to the following quantities:

(1) α/σ

(2, 3) $\mathcal{R}$

(4, 5) LEP prediction of $\mathcal{R}$, $-\alpha(1 - \mathcal{F})/\sigma d$

(6, 7) $-\mathcal{E}_L$

(8, 9) $-\mathcal{F}^\perp$

(10, 11) $-\mathcal{E}_p$

(12, 13) LEP prediction of $-\mathcal{E}_L$, $-(d - 1)(-\alpha/\sigma d - \mathcal{R})$

(14, 15) LEP prediction of $-\mathcal{E}_p$, $d\mathcal{R} + \alpha/\sigma$

(16, 17) $\mathcal{Q}$

(18, 19) $-\mathcal{D}$

(20, 21) λ

(22, 23) κ

(24, 25) EPB prediction of $\mathcal{Q}$, $-(\alpha/\sigma)(\lambda + \kappa)(d - 1)/d$

All properties (except α, which is a parameter) have two columns associated with them, as indicated. The first of the two columns gives the mean value and the second gives the standard error in each case.

The data columns in the `analysed-T1.dat` and `analysed-T125.dat` are exactly the same, except that the number density is prepended to the start of each line, and so each column number is shifted by one.

Figure 2

In this figure, we plot data corresponding to two temperatures, $T/\varepsilon = 1.0$ and $T/\varepsilon = 1.25$, that are provided in the files `analysed-T1.dat` and `analysed-T125.dat`, respectively. The x co-ordinates correspond to column 1 (the number density), and the y co-ordinates correspond to

(a) the orientational response $\mathcal{R}$: columns 3 (simulation data) and 5 (LEP prediction);

(b) the coupling of the rotational kinetic energy to the orientation, $\mathcal{E}_L$: the negative of columns 7 (simulation data) and 13 (LEP prediction);

(c) the correlation of the force and the orientation $\mathcal{Q}$: columns 17 (simulation data) and 25 (EPB prediction).

Figure 3

In this figure, we plot (a) the orientational response as a function of α and (b) a test of the torque-balance condition. The data plotted are provided in the file `analysed-alpha.dat`. The x co-ordinates correspond to column 1 (the value of α/σ), and the y co-ordinates correspond to

(a) the orientational response $\mathcal{R}$: columns 2 (simulation data) and 4 (LEP prediction);

(b) the coupling of the rotational kinetic energy to the orientation, $\mathcal{E}_L$ is the negative of column 6, and the projection of the interparticle force perpendicular to the orientation, $\mathcal{F}^\perp$, is the negative of column 8.

Figure 4

In this figure, we plot deviations from the LEP prediction as a function of α. The data plotted are provided in the file `analysed-alpha.dat`. The x co-ordinates correspond to column 1 (the value of α/σ), and the y co-ordinates correspond to

(a) the coupling of the rotational kinetic energy to the orientation, $\mathcal{E}_L$: the negative of columns 6 (simulation data) and 12 (LEP prediction);

(b) the coupling of the translational kinetic energy to the orientation, $\mathcal{E}_p$: the negative of columns 10 (simulation data) and 14 (LEP prediction);

(c) the correlation between force and orientation $\mathcal{Q}$ is column 16, and the correlation between translational and angular momentum $\mathcal{D}$ is the negative of column 18.

Figure 5

In this figure, we plot predictions from the EPB theory as a function of α. The data plotted are provided in the file `analysed-alpha.dat`. The x co-ordinates correspond to column 1 (the value of α/σ), and the y co-ordinates correspond to

(a) the value of κ: column 22; the value of λ: column 20;

(b) the correlation between force and orientation $\mathcal{Q}$: columns 16 (simulation data) and 24 (EPB prediction).