MS-UCG simulations for the heterogeneous system

Jaehyeok Jin

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1 System description

Uploaded codes in GitHub are designed to simulate the system with heterogeneous systems. To start with the simplest example, let's say the system is composed of two particles: one (particle A) shows the MS-UCG behavior, which is dependent on the local density and the other one (particle B) acts like a normal CG particle. To simulate this behavior in LAMMPS, three particle states are needed.

2 Changes

In the data file, the first and the second particles correspond to MS-UCG behavior and the third particle is a normal CG particle. Also, in here, we suppose particle A interacts strongly with particle A but not with particle B. In order to acheive this, I've switched the probability function for the state 1 with state 2, i.e.

$$P_{i,1} = -\frac{1}{2}\big(\tanh(\frac{w_i - c}{0.1c} - 1\big)$$
$$P_{i,2} = +\frac{1}{2}\big(\tanh(\frac{w_i - c}{0.1c} + 1\big)$$

Thus, the state 1 corresponds to less dense state (low w_i value), the state 2 corresponds to more dense state (high w_i value). A switch between the state 1 and 2 happens in LAMMPS simulation, but all particles are labeled as "1" in the data file, which means particle 1 and 3 interacts weakly.

In the force subroutine in the code, the w_i value is counted only if type$_i$ = 1 and type$_j$ = 1. The MS-UCG force is computed the four subforces only if type$_i$ = 1 and type$_j$ = 1. Instead, normal Lennard-Jones force is computed when type$_i$ = 3 or type$_j$ = 3.

Finally, I've changed the **type linked** (the linked list) function to while loop because the particle 3 doesn't have any state-dependency. I also checked that the newly-implemented while loop successfully describes the state change, i.e. $(\alpha, \beta) = (1,1), (1,2), (2,1), (2,2)$

3 Note

To validate the current code, I've checked the force component with four small systems at the timestep $= 0$ and it shows the identical component compared to the results from LAMMPS. MATLAB code that I used to check the force component is uploaded in GitHub.