Manual for running the BD Codes

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Instructions for Running the Codes Stored in Folder: langevin_dynamics_vs_fokker_plank_equation

This section demonstrates the time evolution of a particle distribution governed by Langevin stochastic dynamics. The corresponding LAMMPS input file for this exercise is `langevin.in`.

System Configuration

The following steps describe how the system is configured in the LAMMPS input script. For additional details on related concepts, students are encouraged to consult Section 1 of the DPD chapter in the LAMMPS manual.

1. **Creating particles in a localized region inside a large simulation box:**

```
region my_box block 0 20 0 20 0 20
create_box 1 my_box

region my_region block 10 11 10 11 10 11
create_atoms 1 random 1000 8009 my_region
```

   A large simulation box is first defined, after which particles are created within a small subregion of the box. This setup effectively corresponds to a delta-function-like initial condition for the particle density at time $t = 0$.

2. **Disabling inter-particle interactions:**

```
pair_style none
```

   Inter-particle interactions are switched off so that the particles behave as ideal, non-interacting diffusive particles at all length scales. This ensures smooth diffusive spreading of the particle distribution. If interactions were enabled, particles could experience transient caging effects, leading to subdiffusive behavior at short times.

3. **Applying a thermostat and an integrator:**

```
fix my_thermo_stat all langevin 1.0 1.0 0.1 89080
fix your_integrator all nve
```

The Langevin thermostat is applied using the `fix langevin` command. This introduces stochastic and frictional forces that maintain the system at a constant temperature. However, the Langevin thermostat alone does not integrate the equations of motion. Therefore, a separate time integrator is required.

In this example, the simple `nve` integrator is used. Since temperature control is already provided by the Langevin thermostat, using an additional thermostat-based integrator (such as `nvt`, which employs a Nose-Hoover thermostat) would result in redundant or conflicting thermostatting.

For systems involving finite-sized particles with rotational degrees of freedom, an appropriate integrator (e.g., `rigid/small`) would be required. In general, the choice of thermostat and integrator must be physically consistent with each other and with the system being simulated.

Steps to Follow

To analyze the time evolution of the particle distribution and compare discrete and continuum descriptions, students should follow the steps below:

1. Run the LAMMPS input script located in the file `langevin.in`.
2. Open OVITO and load the trajectory file `simulation_data.lammpstrj`.
3. Apply the *Histogram* modifier in OVITO and observe the evolution of the particle distribution along the x-direction.
4. Compare the distribution obtained from the Langevin simulation with the solution of the Fokker-Planck equation shown in the animated file `fokker_planck_evolution.gif`. This animation is generated using the Python script `evolution_focker_planck.py`.
5. Observe that the stochastic particle-based Langevin dynamics reproduces the same macroscopic evolution predicted by the continuum Fokker-Planck equation, demonstrating the consistency between the discrete and continuum descriptions.