PHYS 516: Methods of Computational Physics
ASSIGNMENT 4- Molecular Dynamics Simulation

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February 16, 2017

The purpose of this assignment is to get familiar with basic concepts in ordinary differential equations using a simple molecular dynamics (MD) program, *md.c*, as an example.

1 Liouville Theorem

Here, we show that for a particle in 1-D space, the velocity Verlet algorithm exactly preserves the phase space volume for arbitrary time discretization unit, Δ.

Let x be the position of the particle, $p = mv$ the momentum where, m and v are the mass and velocity of the particle. In the dimensionless form, $p = v$. Let the coordinate and momentum of the particle at time t be (x, p), and those at time $t + \Delta$ be (x', p')

$$x' = x + p\Delta + \frac{1}{2}a(x) + \Delta^2 \tag{1}$$

$$p' = p + \frac{a(x) + a(x')}{2}\Delta \tag{2}$$

To show this, it is enough to show that the Jacobian of the transformation $(x'(x, p), p'(x, p))$ is 1, i.e. $J = \left|\frac{\partial(x', p')}{\partial(x, p)}\right| = 1$. The derivatives are calculated from Eq (1) and (2) as follows:

$$\frac{\partial x'}{\partial x} = 1$$
$$\frac{\partial x'}{\partial p} = \Delta$$
$$\frac{\partial p'}{\partial x} = 0$$
$$\frac{\partial p'}{\partial p} = 1$$

Therefore, the Jacobian is given by

$$J = \begin{vmatrix} \frac{\partial x'}{\partial x} & \frac{\partial p'}{\partial x} \\ \frac{\partial x'}{\partial p} & \frac{\partial p'}{\partial p} \end{vmatrix} \tag{3}$$

$$= \begin{vmatrix} 1 & 0 \\ \Delta & 1 \end{vmatrix} \tag{4}$$

$$= 0 \tag{5}$$

2 Comparison of Euler and Velocity-Verlet Algorithms

Total energy of the system should be conserved. But due to numerical errors, energy conservation depends on the time-integration algorithm used. In this section, we illustrate this by comparing the Euler and Velocity-Verlet algorithms.

Euler Algorithm

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Given a configuration $(\boldsymbol{r}_i(t), \boldsymbol{v}_i(t) | i = 1 \text{ to } N_{atom})$
1. Compute the acceleration: $\boldsymbol{a}_i(t)$
2. Update the positions: $\boldsymbol{r}_i(t + \Delta) \leftarrow \boldsymbol{r}_i(t) + \boldsymbol{v}_i(t)\Delta + \frac{1}{2}\boldsymbol{a}_i(t)\Delta^2$
3. Update the velocities: $\boldsymbol{v}_i(t + \Delta) \leftarrow \boldsymbol{v}_i(t) + \boldsymbol{a}_i(t)\Delta$
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Velocity-Verlet Algorithm

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Given a configuration $(\boldsymbol{r}_i(t), \boldsymbol{v}_i(t) | i = 1 \text{ to } N_{atom})$
1. Compute the acceleration: $\boldsymbol{a}_i(t)$
2. $\boldsymbol{v}_i(t + \frac{\Delta}{2}) \leftarrow \boldsymbol{v}_i(t) + \boldsymbol{a}_i(t)\frac{\Delta}{2}$
3. $\boldsymbol{r}_i(t + \Delta) \leftarrow \boldsymbol{r}_i(t) + \boldsymbol{v}_i(t + \frac{\Delta}{2})\Delta$
4. Compute the updated acceleration: $\boldsymbol{a}_i(t + \Delta)$
5. $\boldsymbol{v}_i(t + \Delta) \leftarrow \boldsymbol{v}_i(t + \frac{\Delta}{2}) + \boldsymbol{a}_i(t + \Delta)\frac{\Delta}{2}$
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