

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

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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')

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

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

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:

$$\begin{aligned} \frac{\partial x'}{\partial x} &= 1 \\ \frac{\partial x'}{\partial p} &= \Delta \\ \frac{\partial p'}{\partial x} &= 0 \\ \frac{\partial p'}{\partial p} &= 1 \end{aligned}$$

Therefore, the Jacobian is given by

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

$$= \begin{vmatrix} 1 & 0 \\ \Delta & 1 \end{vmatrix} \quad (4)$$

$$= 1 \quad (5)$$

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.