PHYS 516
Assignment 4
Isabella Johansson
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1. Louisville's theorem.

1. Let the coordinate & momentum of a particle at time t be (x, p), & those in time $t + \Delta$ to be (x', p'). Let $p = mv = v$, or $m = 1$.

The velocity verlet algorithm is:

$$x' = x + \Delta v + \frac{1}{2}\Delta^2 a = x + v\left(t + \frac{\Delta}{2}\right)\Delta \quad (1)$$

$$v\left(t + \frac{\Delta}{2}\right) = v + \frac{1}{2} a \Delta \quad (2)$$

$$v' = v\left(t + \frac{\Delta}{2}\right) + \frac{1}{2} a' \Delta = v + \frac{a + a'}{2}\Delta \quad (3)$$ where a & a' only dep. on x, x'

Now, to show that that this algotritm exacly preserves the phase space volume we show that the Jacobian is 1.

The Jacobian is
$$J(x', v') = \begin{vmatrix} \partial x'/\partial x & \partial x'/\partial v \\ \frac{\partial v'}{\partial x} & \frac{\partial v'}{\partial v} \end{vmatrix} = \frac{\partial x'}{\partial x}\frac{\partial v'}{\partial v} - \frac{\partial v'}{\partial x}\frac{\partial x'}{\partial v} \quad (4)$$

From (1) and (3)

$$\frac{\partial x'}{\partial x} = 1 + 0 + \frac{1}{2}\frac{\partial a}{\partial x}\Delta^2 = 1 + \frac{1}{2}\frac{\partial a}{\partial x}\Delta^2 \quad (5)$$

$$\frac{\partial x'}{\partial v} = \Delta \quad (6)$$

$$\frac{\partial v'}{\partial x} = \frac{1}{2}\left(\frac{\partial a}{\partial x} + \frac{\partial a}{\partial x'}\frac{\partial x'}{\partial x}\right)\Delta = \frac{1}{2}\frac{\partial a}{\partial x} + \frac{1}{2}\frac{\partial a}{\partial x'}\left(1 + \frac{1}{2}\frac{\partial a}{\partial x}\Delta^2\right)\Delta \quad (7)$$

$$\frac{\partial v'}{\partial v} = 1 + \frac{1}{2}\frac{\partial a}{\partial x'}\frac{\partial x'}{\partial v}\Delta = 1 + \frac{1}{2}\frac{\partial a}{\partial x'}\Delta^2 \quad (8)$$

plugging in (5)-(8) into 4 we get

$$J(x', v') = \left(1 + \frac{1}{2}\frac{\partial a}{\partial x}\Delta^2\right)\left(1 + \frac{1}{2}\frac{\partial a}{\partial x'}\Delta^2\right) - \frac{1}{2}\left(\frac{\partial a}{\partial x} + \frac{\partial a}{\partial x'}\left(1 + \frac{1}{2}\frac{\partial a}{\partial x}\Delta^2\right)\Delta\right)(\Delta)$$
$$= 1 + \frac{1}{2}\left(\cancel{\frac{\partial a}{\partial x}} + \cancel{\frac{\partial a}{\partial x'}}\right)\Delta^2 + \cancel{\frac{1}{4}\frac{\partial a}{\partial x}\frac{\partial a}{\partial x'}\Delta^4} - \cancel{\frac{1}{2}\frac{\partial a}{\partial x}\Delta^2} - \frac{1}{2}\cancel{\frac{\partial a}{\partial x'}\Delta^2} - \frac{1}{4}\frac{\partial a}{\partial x}\cancel{\frac{\partial a}{\partial x'}\Delta^4} = 1$$

2. Velocity autocorrelation.

(i) (See modified *md-vac.c* & *md-vac.h* attached separately)
(ii) Plot Z(t)

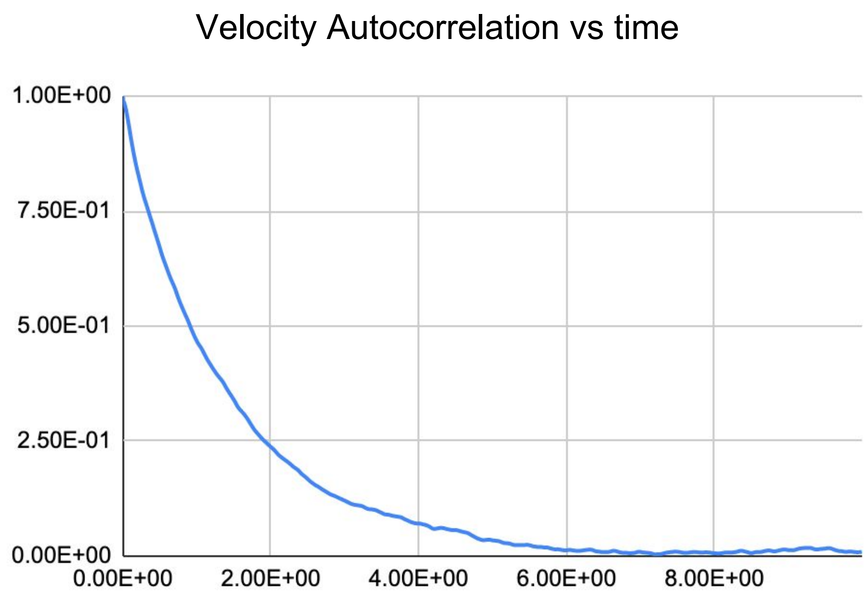

Figure 1. Gas Phase: (Density = 0.1, Temperature = 1.0)

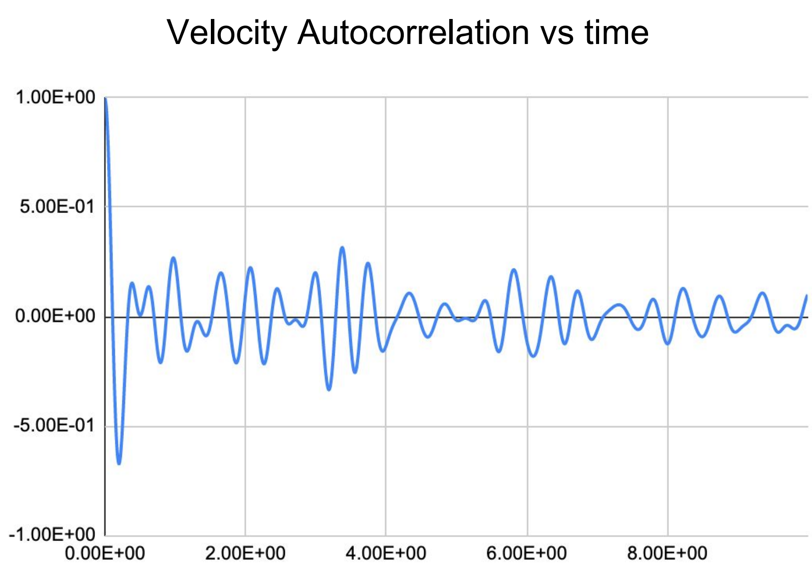

Figure 2. Solid Phase: (Density = 1.0, Temperature = 0.1)

3. Split-operator formalism

3. The Liouville formulation operator: $iL = \sum_{\alpha=1}^{3N} \left[\frac{\partial \mathcal{H}}{\partial p_\alpha} \frac{\partial}{\partial q_\alpha} - \frac{\partial \mathcal{H}}{\partial q_\alpha} \frac{\partial}{\partial p_\alpha} \right]^{(1)}$ where $\mathcal{H}$ is the hamiltonian & $\Gamma = \{x_\alpha, p_\alpha\}$ are position & momentum of the system.

the classical propagator then is $U(t) = e^{iLt}$ (2) & the state of the system at any time t: $\Gamma(t) = U(t)\Gamma(0)$ (3)

Using a choice for $\Gamma(t) = x(t) \rightarrow x_t = e^{iLt} x_0$ (4), now, we seperate iL into two terms: $iL = iL_1 + iL_2$ such that $iL_1 = \sum_{\alpha=1}^{N} \frac{\partial \mathcal{H}}{\partial p_\alpha} \frac{\partial}{\partial q_\alpha}$ & $iL_2 = -\sum_{\alpha=1}^{N} \frac{\partial \mathcal{H}}{\partial q_\alpha} \frac{\partial}{\partial p_\alpha}$ (5)

where $iL_1 iL_2 \phi(x) \neq iL_2 iL_1 \phi(x)$ (6)

using Liouville operator: $\mathcal{H} = \frac{p^2}{2m} + U(x) \rightarrow iL_1 = \frac{p}{m} \frac{\partial}{\partial x}$ & $iL_2 = F(x) \frac{\partial}{\partial p}$ (7)

So that $F(x) = -\frac{dU}{dx}$ (8) (iL_1 & iL_2 doesnt commute)

Now, using the Trotter expansion: $[A,B] \neq 0$ $e^{A+B} = \lim_{P \to \infty} \left[e^{B/2P} e^{A/P} e^{B/2P} \right]^P$ (9)

but for $iL = iL_1 + iL_2$:

$e^{iLt} = e^{(iL_1 + iL_2)t} = \lim_{P \to \infty} \left[e^{iL_2 t/2P} e^{iL_1 t/P} e^{iL_2 t/2P} \right]^P$ (10)

the discrete time propagator is defined as:

$G(\Delta t) = U_1(\Delta t/2) U_2(\Delta t) U_1(\Delta t/2)$ (11) $\Delta t = (t/P) \rightarrow$ discrete time step

using eqn (7) we can write: $G(\Delta t) = e^{(\Delta t/2) F(x) \partial/\partial p} e^{\Delta t \dot{x} \partial/\partial x} e^{(\Delta t/2) F(x) \partial/\partial p}$ (12)

since $P = t/\Delta t$, the error of L goes Δt^2

leading to the propagator: $e^{c\,\partial/\partial q} f(q) = f(q+c)$ (13)

$\Gamma(0) = \{x(0), p(0)\} \rightarrow \Gamma(\Delta t) = U_1\left(\frac{\Delta t}{2}\right) U_2(\Delta t) U_1\left(\frac{\Delta t}{2}\right) \Gamma(0) = \Gamma_1\left(\frac{\Delta t}{2}; \Gamma_2\left(\Delta t; \left[\frac{\Delta t}{2}; \Gamma(0)\right]\right)\right)$

Now, $\{x(\Delta t), p(\Delta t)\} = \{x, p\}_1 \left(\Delta t/2 ; \{x, p\}_1 \left[\frac{\Delta t}{2} ; x(0), p(0) \right] \right\})$

taking eqn (13)

$$\left(x(\Delta t), p(\Delta t)\right) = \left(x(0) + \frac{\Delta t}{m} p(0) + \frac{(\Delta t)^2}{2m} F(x(0))\right), \left(p(0) + \frac{\Delta t}{2}\left(F(x_0) + F(x(\Delta t))\right)\right)$$

$$\therefore \boxed{\begin{aligned} x(\Delta t) &= x(0) + \dot{x}(0)\Delta t + \frac{(\Delta t)^2}{2} \frac{F(x(0))}{m} \\ \dot{x}(\Delta t) &= \dot{x}(0) + \frac{\Delta t}{2m}\left(F(x(0)) + F(x\Delta t)\right) \end{aligned}}$$