M6MD1

1.1) $\underline{p} = \sum_{i=1}^{N} \underline{p}_i$ if $\frac{d\underline{p}}{dt} = 0$ p is constant

$$\frac{d\underline{p}}{dt} = \sum_{i=1}^{N} \frac{d\underline{p}_i}{dt} = \sum_{i=1}^{N} m\underline{a}_i = \sum_{i=1}^{N} \underline{F}_i$$

Know $-\frac{\partial V_i}{\partial \underline{r}_i} = \underline{F}_i$ where $V_i = \sum_{i \neq j} u_{ij}(\underline{r}_i - \underline{r}_j)$

$$\Rightarrow \frac{d\underline{p}}{dt} = -\sum_{i=1}^{N} \sum_{i \neq j} \frac{\partial u_{ij}(\underline{r}_i - \underline{r}_j)}{\partial \underline{r}_i}$$

$$= -\sum_{i=1}^{N} \sum_{i \neq j} F_{ij} = 0$$

Double sum counts all pairwise forces which cancel

$\Rightarrow$ momentum is conserved

1.2) Leap-Frog

$$\underline{r}_i(t+\delta t) = \underline{r}_i(t) + \underline{v}_i\left(t+\frac{\delta t}{2}\right)\delta t \quad A \qquad \text{and} \qquad \underline{V}_i(t) = \frac{1}{2}\left(\underline{v}_i\left(t+\frac{\delta t}{2}\right) + \underline{v}_i\left(t-\frac{\delta t}{2}\right)\right) \quad B$$

$$\underline{V}_i\left(t+\frac{\delta t}{2}\right) = \underline{v}_i\left(t-\frac{\delta t}{2}\right) + \frac{\delta t}{m_i}\underline{f}_i(t) \quad A$$

position verlet

$$\underline{r}_i(t+\delta t) = 2\underline{r}_i(t) - \underline{r}_i(t-\delta t) + \frac{\delta t^2}{2m_i}\underline{f}_i(t) \quad 1$$

$$\underline{v}_i(t) = \frac{1}{2\delta t}\left(\underline{r}_i(t+\delta t) - \underline{r}_i(t-\delta t)\right) \quad 2$$

Consider substituting $\underline{V}_i(t+\delta t) = \dfrac{\underline{r}_i(t+\delta t) - \underline{r}_i(t)}{\delta t}$

$$\underline{V}_i(t-\delta t) = \frac{\underline{r}_i(t) - \underline{r}_i(t+\delta t)}{\delta t}$$

into A

$$\Rightarrow \frac{\underline{r}_i(t+\delta t) - \underline{r}_i(t)}{\delta t} = \frac{\underline{r}_i(t) - \underline{r}_i(t-\delta t)}{\delta t} + \frac{\delta t^2}{m_i}\underline{f}_i(t)$$

$$\Rightarrow \underline{r}_i(t+\delta t) = 2\underline{r}_i(t) - \underline{r}_i(t-\delta t) + \frac{\delta t^2}{m_i}\underline{f}_i(t) = 1$$

Into B $\Rightarrow$ $\underline{v}_i(t) = \frac{1}{2\delta t}\left(\underline{r}_i(t+\delta t) - \cancel{\underline{r}_i(t)} + \cancel{\underline{r}_i(t)} - \underline{r}_i(t-\delta t)\right)$

$$\Rightarrow \underline{v}_i(t) = \frac{1}{2\delta t}\left(\underline{r}_i(t+\delta t) - \underline{r}_i(t-\delta t)\right) = 2$$

$\Rightarrow$ A $\equiv$ 1, B $\equiv$ 2 $\Rightarrow$ Leap frog and Verlet are equivalent

1.3) a) $C_{AA}(\tau) = \langle A(t) A(t+\tau) \rangle$

$$= \langle \cos(\omega t) \cos(\omega(t+\tau)) \rangle$$

$$= \frac{1}{2} \langle \cos(\omega\tau) + \cos(2\omega t + \omega\tau) \rangle$$

$\Delta t \gg \frac{2\pi}{\omega}$

$$= \frac{1}{2} \langle \cos(\omega\tau) \rangle$$

$$= \frac{1}{2} \cos(\omega\tau)$$

b) $C_{AA}(\tau) = \langle (a_1 \cos(w_1 t) + a_2 \cos(w_2 t))(a_1 \cos(w_1(t+\tau)) + a_2 \cos(w_2(t+\tau)))\rangle$

$$= \langle \overset{①}{a_1^2 \cos(w_1 t) \cos(w_1(t+\tau))} + \overset{②}{a_2^2 \cos(w_2 t) \cos(w_2(t+\tau))}$$

$$+ \overset{③}{a_1 a_2 \cos(w_1 t) \cos(w_2(t+\tau))} + \overset{④}{a_2 a_1 \cos(w_2 t) \cos(w_1(t+\tau))}\rangle$$

① $\Rightarrow \langle \frac{a_1^2}{2}\left(\cos(w_1 \tau) + \cancelto{0}{\cos(2w_1 t + w_1\tau)}\right)\rangle = \frac{a_1^2}{2}\cos(w_1 \tau)$

② $\Rightarrow \langle \frac{a_2^2}{2}\left(\cos(w_2 \tau) + \cancelto{0}{\cos(2w_2 t + w_2\tau)}\right)\rangle = \frac{a_2^2}{2}\cos(w_2 \tau)$

③ $\Rightarrow \langle \frac{a_1 a_2}{2}\left(\cancelto{0}{\cos((w_2 - w_1)t + w_2 \tau)} + \cancelto{0}{\cos((w_2+w_1)t + w_2\tau)}\right)\rangle = 0$

④ $\Rightarrow \quad = 0$

$\Rightarrow \quad C_{AA}(\tau) = \frac{a_1^2}{2}\cos(w_1\tau) + \frac{a_2^2}{2}\cos(w_2\tau)$