MULTIPLE-TIME STEP ALGORITHMS

For M.D. we need $\Delta t \ll \tau$ ~ typical time scale of the system

There are systems in which $\vec{F} = \vec{F}_1 + \vec{F}_2$ with

$\vec{F}_1$ time scale τ_1

$\vec{F}_2$ time scale τ_2

$\boxed{\text{with } \tau_1 \ll \tau_2}$

$\vec{F}_1$ fast component

$\vec{F}_2$ slow component

We can speed up the dynamics using two time steps

$\Delta t_2 \ll \tau_2$ (but NOT $\Delta t_2 \ll \tau_1$)

$\Delta t_1 \ll \Delta t_2$ such that $\Delta t_1 \ll \tau_1$

Liouvillian

$$iL = \frac{p}{m}\cdot\frac{\partial}{\partial q} + (\bar{F}_1 + \bar{F}_2)\cdot\frac{\partial}{\partial p} =$$

$$= iL_q + \underbrace{iL_{1p}}_{\text{fast component}} + \underbrace{iL_{2p}}_{\text{slow component}}$$

Define $t = N\Delta t_2$ $\boxed{\dfrac{\Delta t_2}{\Delta t_1} = n}$

$$e^{iLt} = \left(e^{iL\Delta t_2}\right)^N$$ = exact as usual

Now the approximation

$$\text{(A)} \quad e^{iL\Delta t_2} = e^{iL_{2p}\Delta t_2/2}\, e^{i(L_q+L_{1p})\Delta t_2}\, e^{iL_{2p}\Delta t_2/2}$$

This is the usual approximation with

$$L_q \longrightarrow L_q + L_{1p}$$

Now we can use $\Delta t_2 = n\,\Delta t_1$ to rewrite

$$\text{(A)} \quad = e^{iL_{2p}\Delta t_2/2} \left[e^{i(L_q+L_{1p})\Delta t_1} \right]^n e^{iL_{2p}\Delta t_2/2}$$

↑

exact product in terms of steps Δt_1

↓ usual approx.

$$= e^{iL_{2p}\Delta t_2/2} \left[e^{iL_{1p}\Delta t_1/2}\, e^{iL_q\Delta t_1}\, e^{iL_{1p}\Delta t_1/2} \right]^n e^{iL_{2p}\Delta t_2/2}$$

- PRACTICAL IMPLEMENTATION

We start from $r(t)$, $p(t)$

(a) we apply $e^{iL_{2p}\Delta t_2/2}$ and define

$$r_0(t) = r(t)$$

$$p_0(t) = p(t) + \frac{\Delta t}{2} F_2(r(t)) \quad \text{← only the slow component}$$

(b) We perform n steps of time step Δt_1, using only F_1 [standard velocity Verlet update]

$r_0(t')$ and $p_0(t')$ input $\quad [p_0 = m v_0]$

$$r_0(t'+\Delta t_1) = r_0(t') + v_0(t')\Delta t_1 + \frac{\Delta t_1^2}{2m}(F_1(t'))$$

$$v_0(t'+\Delta t_1) = v_0(t') + \frac{\Delta t_1}{2m}(F_1(t') + F_1(t'+\Delta t_1))$$

After n steps we obtain

$r_0(t+n\Delta t_1)$ and $p_0(t+n\Delta t_1)$ $\boxed{n\Delta t_1 = \Delta t_2}$

(c) We apply again $e^{iL_{2p}\Delta t_2/2}$

$$\begin{cases} r(t+\Delta t_2) = r_0(t+n\Delta t_1) \\ p(t+\Delta t_2) = p_0(t+n\Delta t_1) + \dfrac{\Delta t}{2} F_2(r_0(t+n\Delta t_1)) \end{cases}$$

only the slow component

Computational advantage:

At each time step Δt_2 we compute

- $F_1(r)$ n times
- $F_2(r)$ only <u>once</u> $[F_2(r(t+\Delta t_2))]$