Numerische Integration der Bewegungsgleichungen:

$m\ddot{\underline{r}}_i = \underline{F}_i$ (Newton)

$\underline{r}(t \pm \Delta t) = \underline{r}(t) \pm \Delta t\, \dot{\underline{r}}(t) + \frac{\Delta t^2}{2} \ddot{\underline{r}}(t) \pm O(\Delta t^3)$

$\underline{r}(t+\Delta t) + r(t-\Delta t) = 2\underline{r}(t) + \Delta t^2 \ddot{\underline{r}}(t) + O(\Delta t^4)$

$\boxed{\underline{r}(t+\Delta t) = 2\underline{r}(t) - \underline{r}(t-\Delta t) + \Delta t^2 \frac{\underline{F}(t)}{m}} \cancel{+ O(\Delta t^4)}$

Verlet - Algorithmus

Geschwindigkeiten kommen nicht vor!

$\dot{\underline{r}}(t+\Delta t) = \dot{\underline{r}}(t) +$

$\dot{\underline{r}}(t) = \frac{\underline{r}(t+\Delta t) - \underline{r}(t-\Delta t)}{2\Delta t}$

Leap-frog

$\underline{r}(t+\Delta t) = \underline{r}(t) + \Delta t\, \dot{\underline{r}}(t + \frac{\Delta t}{2})$

$\dot{\underline{r}}(t + \frac{\Delta t}{2}) = \dot{\underline{r}}(t - \frac{\Delta t}{2}) + \Delta t\, \ddot{\underline{r}}(t) = \dot{\underline{r}}(t - \frac{\Delta t}{2}) + \frac{\Delta t}{m} \underline{F}(t)$

$\dot{\underline{r}}(t) = \frac{1}{2}\left(\dot{\underline{r}}(t - \Delta t/2) + \dot{\underline{r}}(t + \frac{\Delta t}{2})\right)$

$\cancel{\underline{r}(t+\Delta t) = \underline{r}(t) + \Delta t \frac{1}{2} \dot{\underline{r}}(t - \Delta}$

Äquivalenz Verlet – Leapfrog:

$$r(t \pm \Delta t) = r(t) \pm \Delta t\, \dot{r}(t \pm \tfrac{\Delta t}{2})$$

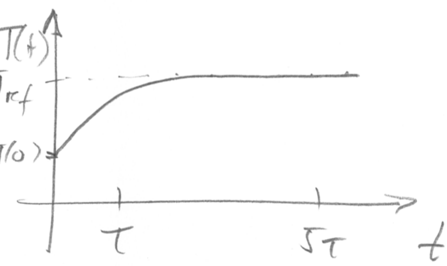
$$\dot{r}(t + \tfrac{\Delta t}{2}) = \dot{r}(t - \tfrac{\Delta t}{2}) + \Delta t\, \ddot{r}(t)$$

$$\begin{aligned} r(t+\Delta t) &= r(t) + \Delta t\, \dot{r}(t - \tfrac{\Delta t}{2}) + \Delta t^2 \ddot{r}(t) \\ &= r(t) + r(t) - r(t-\Delta t) + \Delta t^2 \ddot{r}(t) \\ &= 2r(t) - r(t-\Delta t) + \Delta t^2 \ddot{r}(t) \end{aligned}$$

Verlet! ∎

Schwache Kopplung an ein Wärmebad:

$$T(t) = T_{ref} + \left(T(0) - T_{ref}\right) e^{-t/\tau}$$



$$\frac{dT}{dt} = \frac{\left(T(0) - T_{ref}\right) e^{-t/\tau}}{-\tau} = \frac{T_{ref} - T(t)}{\tau}$$

Skalierung des Geschwindigkeiten in jedem Zeitschritt, Δt:

$$\underline{v}_i \longrightarrow \underline{v}_i^{new} = \lambda \underline{v}_i$$

$$\Delta E_{kin} = \sum_i \frac{1}{2} m_i \left(\underline{v}_i^{new}\right)^2 - \sum_i \frac{1}{2} m_i \underline{v}_i^2$$

$$= \left(\lambda^2 - 1\right) \sum_i m_i \underline{v}_i^2 = \left(\lambda^2 - 1\right) E_{kin}$$

$$E_{kin} = \frac{N k_B T}{2} \implies \Delta T = \left(\lambda^2 - 1\right) T$$

$$\frac{T_{ref} - T(t)}{\tau} = \frac{dT}{dt} \simeq \frac{\Delta T}{\Delta t} = \left(\lambda^2 - 1\right) \frac{T(t)}{\Delta t}$$

$$\lambda^2 - 1 = \frac{\Delta t}{\tau} \frac{T_{ref} - T(t)}{T(t)} \implies \boxed{\lambda = \sqrt{1 + \frac{\Delta t}{\tau} \frac{T_{ref} - T(t)}{T(t)}}}$$

Skalierung des Geschwindigkeiten in jedem Zeitschritt mit Faktor λ liefert exponentielle Anpassung an Referenztemperatur T_{ref}.

Schwache Kopplung für Druck

$$\frac{dP}{dt} = \frac{P_{ref} - P(t)}{\tau_p}$$

Skalierung der Positionen $\underline{r}_i^{new} \longrightarrow \mu \underline{r}_i$

des Volumens $V^{new} \longrightarrow \mu^3 V$

Ideales Gas: $pV = Nk_BT$

$$P^{new} = \frac{Nk_BT}{V^{new}} = \frac{Nk_BT}{\mu^3 V} = \frac{1}{\mu^3} P$$

$$\Delta P = P^{new} - P = \left(\frac{1}{\mu^3} - 1\right) P$$

$$\frac{P^{ref} - P(t)}{\tau_p} = \frac{dP}{dt} \approx \frac{\Delta P}{\Delta t} = \frac{P}{\Delta t}\left(\frac{1}{\mu^3} - 1\right)$$

$$\frac{1}{\mu^3} - 1 = \frac{\Delta t}{\tau_p} \cdot \frac{P^{ref} - P(t)}{P(t)}$$

$$\mu = \frac{1}{\sqrt[3]{1 + \frac{\Delta t}{\tau_p} \frac{P^{ref} - P(t)}{P(t)}}} \simeq \sqrt[3]{1 - \frac{\Delta t}{\tau_p} \frac{P_{ref} - P(t)}{P(t)}}$$

$$\frac{1}{1+x} \simeq 1 - x \quad , \text{falls } |x| \ll 1$$