Overdamped Langevin eq.

$$\dot{x}(t) = -\Gamma \partial_x U + \eta = +\Gamma F(x) + \eta$$

$$\langle \eta(t)\, \eta(t') \rangle = 2\Gamma k_B T \;\delta(t-t')$$

Heun algorithm

discretize the time with time steps τ

at time t the system is in x_t

$$\eta_t = \sqrt{2\Gamma k_B T \tau}\;\xi \qquad ; \xi \text{ drawn from } P(\xi) = \frac{e^{-\left(\frac{\xi^2}{2}\right)}}{\sqrt{2\pi}}$$

$$z = x_t + \tau \Gamma F(x_t) + \eta_t \leftarrow \text{same noise}$$

$$x_{t+1} = x_t + \frac{\tau}{2}\Gamma\Big(F(x_t) + F(z)\Big) + \eta_t$$

with multiplicative noise

$$\dot{x}(t) = f(x) + b(x)\,\xi(t) \qquad \langle \xi \xi' \rangle = 2\,\delta(t-t')$$

$$z = x_t + \tau f(x_t) + b(x_t)\,\xi$$

$$x_{t+1} = x_t + \frac{\tau}{2}\Big(f(x_t) + f(z)\Big) + \frac{\sqrt{\tau}}{2}\Big(b(z) + b(x_t)\Big)\xi$$

$$\dot{x} = \frac{p}{m}$$

$$\dot{p} = -\partial_x U - \gamma \frac{p}{m} + \eta(t) \; ; \; \langle \eta \eta' \rangle = 2\gamma k_B T \delta(t-t')$$

$$x_t \, , \; v_t = \frac{p_t}{m}$$

$$x_{t+\frac{1}{2}} = x_t + v_t \frac{\tau}{2}$$

$$\eta_t = \sqrt{2\gamma k_B T \tau} \; \xi$$

$$v_{t+1} = c_2 \left(v_t \cdot c_1 + F(x_{t+\frac{1}{2}}) \cdot \frac{\tau}{m} + \frac{\eta_t}{m} \right)$$

$$x_{t+1} = x_{t+\frac{1}{2}} + v_{t+1} \frac{\tau}{2}$$

$$c_1 = 1 - \frac{1}{2} \frac{\gamma \tau}{m} \; ; \; c_2 = \frac{1}{1 + \frac{1}{2} \frac{\gamma \tau}{m}}$$

$$v_t + \left(F(x_{t+\frac{1}{2}}) - v_t \gamma \right) \frac{\tau}{m} + \sqrt{2\gamma k_B T \tau} \; \xi$$

$$+ \left(\frac{v_t \gamma^2 - F\left(x_{t+\frac{1}{2}}\right) \gamma}{2m^2} \right) \tau^2 - \frac{\gamma}{2m^2} \tau \sqrt{2\gamma k_B T \tau} \; \xi + O(\tau^{\frac{5}{2}})$$