Computer Science II
L3: SDE / τ-leaping

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Recap SDE

- Remember that a Stochastic Differential Equation (SDE) can be modeled as follows:

$$\underbrace{dX(t)}_{\substack{\textbf{Change of state}}} = \underbrace{a(X,t)dt}_{\substack{\textbf{Deterministic} \\ \textbf{component} \\ \text{(drift)}}} + \underbrace{b(X,t)dW}_{\substack{\textbf{Stochastic} \\ \textbf{component} \\ \text{(diffusion)}}}$$

Euler-Maruyama

- We can use the **Euler-Maruyama** method to numerically solve and simulate the system of SDEs:

$$X(t+\Delta t) = X(t) + a(X(t),t)\cdot\Delta t + b(X(t),t)\cdot\sqrt{\Delta t}\cdot\mathcal{N}(0{,}1)$$

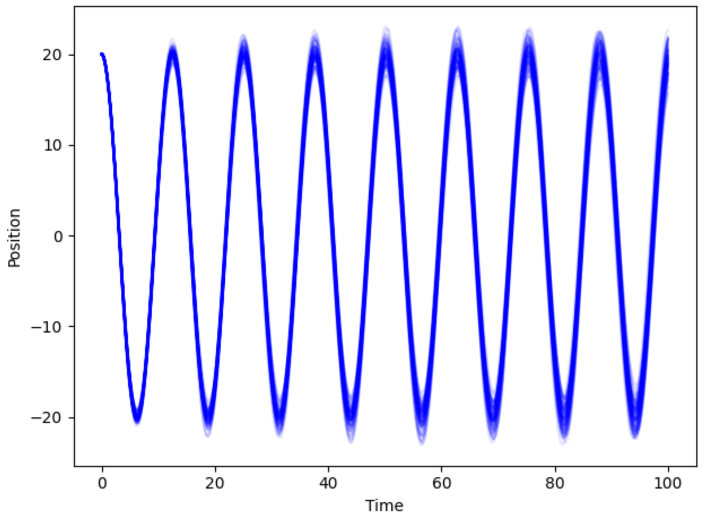
- Δt is the **step size**
- $\mathcal{N}(0{,}1)$ is a random number sampled from a **standard Gaussian distribution**

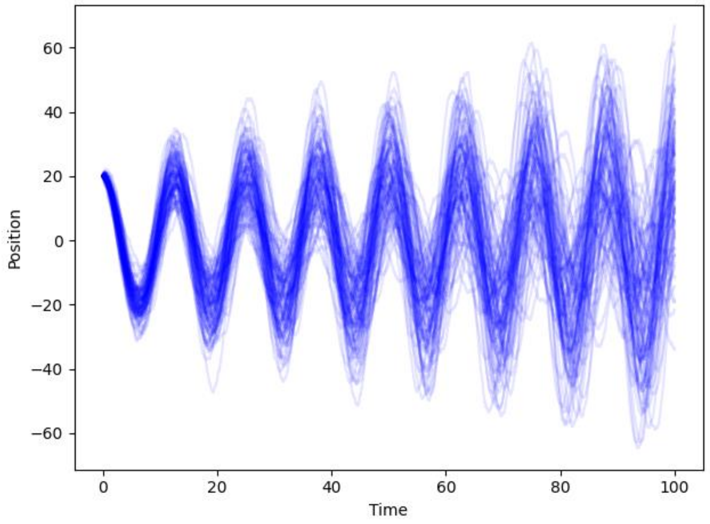
Toy exercise: stochastic oscillator

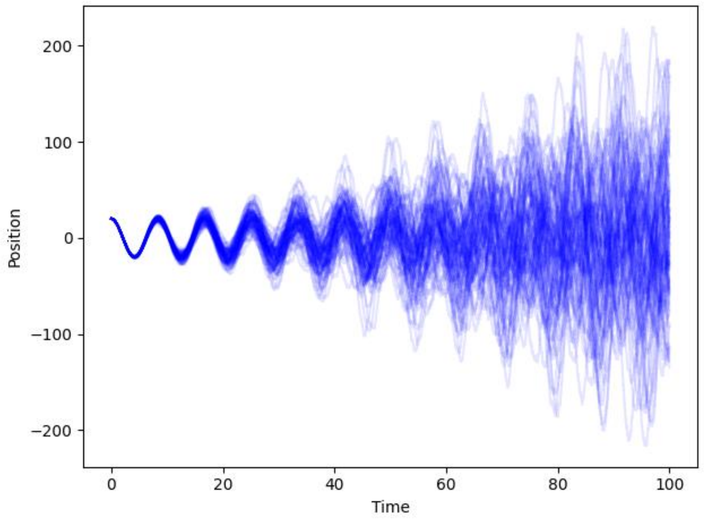
- Get back to the example of **Harmonic Oscillator** (HO)
  - Consider a **stochastic variant** of HO in which the collisions with particles introduce a **small amount of noise**
  - Forget about the physical meaning for a while, this is just an exercise

- Take back the HO equations that we saw in the previous lab
- Introduce **additive noise terms** in both the velocity and position ODEs
- Experiment with the **behavior** of the system, play with **parameters**, check what happens with different b functions (e.g., time-dependent)

Possible results







Adaptive τ-leaping

- Implement a very simple variant of the τ-leaping algorithm with **adaptive step size**. It should work as follows:
  1. The user specifies a τ_0 value, a r_tol "relative tolerance" value, and t_{max}
  2. Calculate all propensities
  3. The algorithm performs a step using step size τ
  4. If the state is not valid (e.g., negative amounts) set $\tau = \tau/2$ and go to step 3
  5. Calculate the new propensities
  6. Calculate the relative change of all propensities (see next slide)
  7. If the mean of all relative changes is greater than r_tol set $\tau = \tau/2$ and go to step 3
  8. Update the system state, reset $\tau = \tau_0$
  9. If $t > t_{max}$ then halt, else iterate from step 2

Calculating the relative change

- Given a reaction R_j we can calculate the relative change of the associated propensity as:

$$relchange_j = \frac{\left|a_j\big(\mathbf{X}(t+\tau)\big) - a_j\big(\mathbf{X}(t)\big)\right|}{a_j\big(\mathbf{X}(t)\big)}$$

- This is just one way to calculate the change
- Please note that this formula breaks down when $a_j\big(\mathbf{X}(t)\big) = 0$, which can happen with very high probability!