PHYS 805 Quiz 2 (Redo)

1. A is Langevin dynamics since it has both velocity & position terms.
   B is Brownian dynamics since it only has position (negligible velocity)

   ODE for A: $m\frac{dv}{dt} = \xi_x(t)\hat{x} + \xi_y(t)\hat{y} - \xi V$; where $\xi_x = \sqrt{\frac{2K_BT\xi}{\Delta t}}$ radn(1)

   $$\Rightarrow \text{In term of } x: \; m\frac{d^2x}{dt^2} = -\xi\frac{dx}{dt} + \underbrace{\sqrt{2K_BT\xi}\,\text{radn}(1)}_{\text{random noise.}}$$

   ⇒ ODE for B: same with A but ignore velocity term

   $$\Rightarrow \xi\frac{dx}{dt} = \sqrt{2K_BT\xi}\,\text{radn}(1)$$

2. $\frac{\partial c}{\partial t} = 5\frac{\partial c}{\partial x} - \frac{1}{2}c$ ⇒ looks like an advection equation

A. Since it is an advection equation, I think we should use backward difference to calculate spatial derivative since the particle flows from left → right in this case (positive V). Forward difference will need a negative velocity & central depends on the concentration on the right, which is unknown in this case. Backward also ensure the stability condition in this case.

B. Since it is a first order ODE, there's only 1 boundary condition that's needed.

c. For $j = N-2$ & $j = N-1$: $\frac{\partial C}{\partial x} \approx \frac{C^i_j - C^i_{j-1}}{\Delta x}$ (backward difference for spatial deriv)

Previously, for the advection code in the lecture:

```
    if V>=0:
(For)  dC[0] = (C[0, i-1] - C[N-1, i-1])/dx  (Boundary cond.) (1st → last)
(Back) dC[1:N] = (C[1:N, i-1] - C[:N-1, i-1])/dx (BoundCond) (last → 1st)
    else:                              ↑ No need since they're not @ boundary
(For)  dC[:N-1] = (C[1:N, i-1] - C[:N-1, i-1])/dx
(For)  dC[N-1] = (C[0, i-1] - C[N-1, i-1])/dx
```

⇒ Therefore for N-2 & N-1:

```
    if V>=0:
        dc[N-2] = (C[N-2, i-1] - C[N-3, i-1])/dx
        dC[N-1] = (C[N-1, i-1] - C[N-2, i-1])/dx
    else:
        dC[N-2] = (C[N-1, i-1] - C[N-2, i-1])/dx
        dC[N-1] = (C[0, i-1] - C[N-1, i-1])/dx
```