Broken detailed balance at mesoscopic scales in active biological systems

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Introduction

Systems in thermodynamic equilibrium are not only characterized by time-independent macroscopic properties, but also satisfy the principle of detailed balance in the transitions between microscopic configurations. A thermodynamic equilibrium is characterized by the fact that all microscopic states are equally accessible, and the probability of a transition between two states is equal to the probability of the reverse transition.

In contrast, most of living systems are characterized by out of equilibrium scenario and characterized by directed fluxes through chemical states which breaks principle of detailed balance at molecular scale. For instance, metabolic and enzymatic processes drive closed-loop fluxes through the system's chemical states.

Non-equilibrium driving of a system can boost intercellular transport, accuracy of transcription, chemotaxis and accuracy of sensory preception. So to understand the cell function it is important to understand whether the system is in equilibrium or not, which is not a simple task.

In this paper, we'll explore the **probability flux analysis (PFA)** a non invasive method to understand and quantify this broken detailed balance in real, nosiy, mesoscopic sytem.

Model

To understand this approach we'll consider a model 1D bead string model. We'll consider two scenario where we have two beads are attached to heat bath with two beads attached to bath with temperature T_1 and T_2 such that $T_1 \neq T_2$ generating a temperature gradient and hence driving it out of equilibrium. One can also analyse the same situation in equilibrium where $T_1 = T_2$.

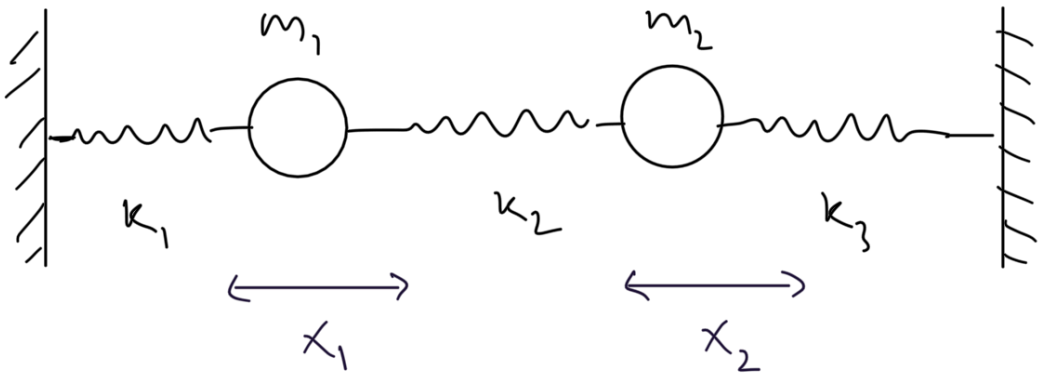

Figure 1: Bead string model

The equation of motion of the above system in lagenvin dynamics system

$$m\frac{\mathrm{d}^2x_1}{\mathrm{d}t^2} = -k_1x_1 - k_2(x_1 - x_2) - \gamma m\frac{\mathrm{d}x_1}{\mathrm{d}t} + \eta_1(t) \tag{1}$$

$$m\frac{\mathrm{d}^2x_2}{\mathrm{d}t^2} = -k_3x_2 - k_2(x_2 - x_1) - \gamma m\frac{\mathrm{d}x_2}{\mathrm{d}t} + \eta_2(t) \tag{2}$$

Now in the overdamped limit we have

$$\gamma\frac{\mathrm{d}x_1}{\mathrm{d}t} = -\frac{k_1}{m}x_1 - \frac{k_2}{m}(x_1 - x_2) + \eta_1(t) \tag{3}$$

$$\gamma\frac{\mathrm{d}x_2}{\mathrm{d}t} = -k_3x_2 - k_2(x_2 - x_1) + \eta_2(t) \tag{4}$$

Dynamics of beads with time

We can numerically solve Eq. 3 and Eq. 4 to get the dynamics of the system using Euler-Maruyama method

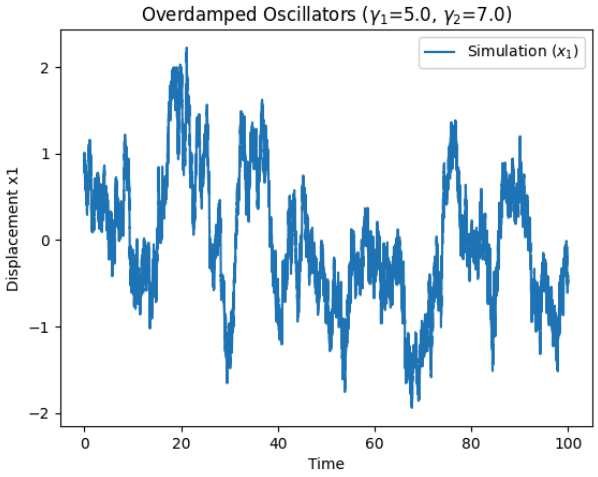

Figure 2: Displacement of bead 1 with time

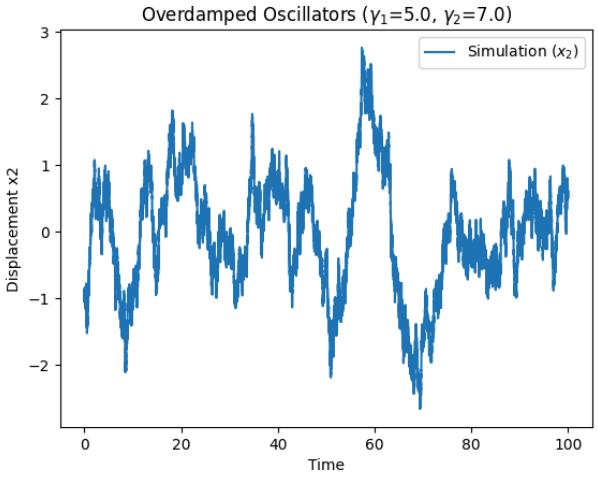

Figure 3: Displacement of bead 2 with time

Probability flux analysis

In equilibrium, systems obey detailed balance—transitions between any two microstates are equally likely in both directions, so there's no net "flow" or flux in phase space. Here is the method to calculate the probability flux in a system.

1. **Define the system state space**
   Choose relevant degrees of freedom, in our case we'll consider the position (x_1) and (x_2) of the beads.
2. **Discretize the State Space**
   Divide the continuous phase space into a coarse-grained grid (called CGPS). Each grid box is a "state bin".
3. **Collect Transitions Between States**
   Track how often the system moves from state/bin $a \to b$ and $b \to a$ and denote these counts as N_{ab} and N_{ba}.
4. **Compute Net Flux**
   Define the net probability flux between bins as:

$$\omega_{ab} = \frac{N_{ab} - N_{ba}}{t} \tag{5}$$

   Flux arrows are plotted from bin $a \to b$ with a length proportional to the net flux ω_{ab}.

Results

Bibliography