Modelling Non-Equilibrium Using Python

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Introduction

At equilibrium, the rates of transition into and out of a system's microstate are balanced. This is to say that the system obeys detailed balance, where each elementary process is equilibrated by its reverse process. Systems that obey detailed balance have transition rates between any two microstates that are pairwise balanced. At equilibrium, in the entire phase space composed of many such microstates, there cannot exist any pair of states which have a net flux between them. Almost all systems found in biology, however, are not in equilibrium, and detailed balance is violated at a molecular scale. Such processes are characterised by the directed fluxes through chemical states. For instance, metabolic and enzymatic processes drive closed-loop fluxes through the system's chemical states. Quantifying the extent to which a system breaks detailed balance is useful, because this characterises the extent to which it deviates from equilibrium.

Overview

In this course we will use computer simulations to study Brownian particles out of equilibrium using the Python programming language. By making use of its scientific computational library, we will simulate one-dimensional and two-dimensional random walks as instances of equilibrium systems and compute the distribution of end positions. Next, we will drive particles by providing a directional bias to the noise, and study differences in the mean squared displacement (MSD). Finally, we will simulate a pair of connected harmonic oscillators, coupled to independent temperature baths. In this system energy is perpetually conducted by a spring from the hot bead to the cold bead. By calculating the flux of probabilities in state space, we will identify signatures of non-equilibrium in this system.

Schedule

Time	Activity	Duration
13h30	Introduction	10min
13h40	Python	40min
14h20	Introduction to Task 1	10min
14h30	Task 1	30min
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15h00	Break	20min
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15h20	Introduction to Task 2	20min
15h40	Task 2	15min
15h55	Introduction to Task 3	30min
16h25	Task 3	∞