Overview of course

Tuesday, January 13, 2009
12:54 AM

No classes or office hours next week.

$$2704 = 3^3 \times 10^2 + 2^2$$

Other references for **rigorous stochastic differential equations:**

Oksendal, Stochastic Differential Equations

Karatzas and Shreve, Brownian Motion and Stochastic Calculus

Gard, Stochastic Differential Equations

A quick look at some of the equations in the models we shall explore:

Statistical Dynamics of Molecules and Particles

Deterministic mechanics of particles:

$\vec{X}$: position of all particles

$\vec{p}$: momenta of all particles

These are each supervectors with 3N components where N is the number of particles in the system.

$$M \frac{d\vec{X}}{dt} = \vec{p}$$

$$\frac{d\vec{p}}{dt} = \underbrace{-\vec{\nabla}\Phi(\vec{X})}_{= \text{force}}$$

M : mass matrix

Φ : potential energy

This becomes unwieldy for microscopic particles in a fluid because the molecular nature of the fluid becomes important by generating Brownian motion and related effects. One way to take care of this in molecular dynamics is to simulate the individual water molecules. This is done but limits the size of the system that can be simulated. An alternative approach is to represent the water molecules statistically. So in the simulation, only the degrees of freedom of the particles or molecules of central interest are simulated, and the effects of the water molecules are treated through the addition of more force terms.

(T. Schlick, Molecular Modeling and Simulation)

stochastic

(T. Schlick, Molecular Modeling and Simulation)

hydrodynamic friction

stochastic thermal forcing

$$m \frac{d\vec{X}}{dt} = \vec{p}$$

$$\frac{d\vec{p}}{dt} = -\vec{\nabla}\Phi(\vec{X}) - \Gamma(\vec{X})\vec{p} + F_T(\vec{X}, t)$$

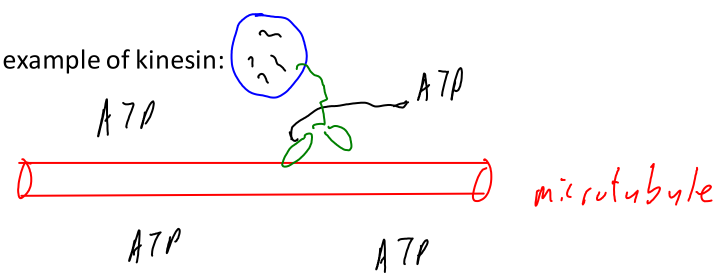
How do I prescribe a physically (and mathematically!) correct description for the thermal forcing? (non-equilibrium statistical mechanics)

Once the thermal forcing is prescribed, how do we describe the resulting dynamics of the particle system?

Molecular Motors

These are devices, either biological or artificial, which are designed to harness thermal energy to do useful work.

Natural example of kinesin:



$\longrightarrow X(t)$

$$0 = -\Gamma \frac{d\vec{X}}{dt} - \vec{\nabla}\Phi(\vec{X}(t), f(t)) + \vec{y}(t) + \vec{F}_T(t)$$

$$\| \quad m\frac{d^2\vec{X}}{dt^2}$$

$$\Gamma \frac{d\vec{X}}{dt} = -\vec{\nabla}\Phi(\vec{X}(t), f(t)) + \vec{y}(t) + \vec{F}_T(t)$$

stochastic processes modeling chemical activation

thermal flucs

Neuroscience

Neurons signal each other essentially through discrete spikes in voltage called action potentials. The dynamics by which a neuron releases and processes these spikes is through the dynamics of its voltage.

$$C\frac{dV}{dt} + g_\ell (V - V_\ell) + g_e(t)(V - V_e) + g_i(t)(V - V_i) = 0$$

V: voltage

C: capacitance

g_ℓ: conductance to leakage

g_e: conductance to excitatory synapses

g_i: conductance to inhibitory synapses

V_ℓ, V_e, V_i: leakage, excitatory, inhibitory voltages