

# Stochastic Mode Reduction: Modern Adaptations and Applications

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12:02 PM

The calculation we've just completed can be understood as one of the simplest examples of the following class of problems:

Suppose we have a system (possibly high-dimensional) of stochastic equations which can be expressed, after an appropriate nondimensionalization, in the following form:

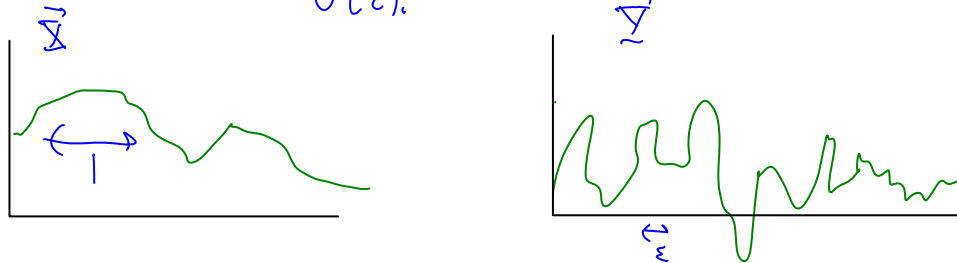
$$d\vec{X} = a(\vec{X}, \vec{Y}, t) dt$$

$$d\vec{Y} = \frac{1}{\epsilon} b(\vec{X}, \vec{Y}, t) dt + \frac{1}{\sqrt{\epsilon}} \sigma(\vec{X}, \vec{Y}, t) d\vec{W}(t)$$

for a small parameter  $\epsilon$

The idea is that the system can be decomposed into a set of slowly evolving variables  $\vec{X}$  and fast variables  $\vec{Y}$

In this nondimensionalization, the time scale of the  $X$  variables is order one while the time scale of the  $Y$  variables is  $O(\epsilon)$ .



We've assumed no noise driving the slow variables, which is the usual case but one could extend to include noise on the slow variables with more work.

Now the project typically is that the full system as stated is very complex and difficult to analyze/compute directly. Certainly the computational simulation would be stiff because of the different time scales of the variables. The question is how can one use the smallness of the time scale ratio between the variables to derive perhaps a simpler effective equation for the slow variables either analytically or through a multiscale computation scheme. That is, we want to do a reduction like that of Klein-Kramers to Smoluchowski for more general systems. That is, we are most interested in simulating the behavior of the slow variables and are willing to coarse-grain information about the fast variables, provided it is done accurately enough so their influence on the slow variables are accurately represented. The noise on the fast variables typically reflects input to the system that's essentially impossible to model in any detail other than statistical to begin with.

The mathematical ideas behind these reductions go back to the 1960s and 1970s, associated with [Khasminskii](#) and [Tom Kurtz](#). They have been revived in the last 10 years or so because of realization of how they can be used in computational contexts.

Examples:

First a classical case from the 1970s which was done through analytical techniques. Can we describe Brownian motion from starting with a detailed molecular model for both the fluid and the microscale particle.



The fluid molecules and the large solvent molecule are described by some Hamiltonian dynamics based on certain force laws between them (hard sphere collisions, etc.) The question then is, starting with a system of many differential equations keeping track

of the positions and velocities of all the fluid particles and the solvent particle, can we derive an effective equation for the solvent particle and show that it looks like Brownian motion.

$$\Phi(\vec{X}, \vec{Y}^{(1)}, \vec{Y}^{(2)}, \dots)$$

↑ solvent position
↑ water positions

$$\frac{d\vec{X}}{dt} = \vec{V}$$

$$M \frac{d\vec{V}}{dt} = - \vec{\nabla}_{\vec{X}} \Phi$$

$$\frac{d\vec{Y}^{(j)}}{dt} = \vec{V}^{(j)}$$

$$m \frac{d\vec{V}^{(j)}}{dt} = - \vec{\nabla}_{\vec{Y}^{(j)}} \Phi$$

One hopes to reduce this high-dimensional system (with many fluid molecules) to a single vector stochastic differential equation for the position  $\vec{X}$  of the solvent molecule, coarse graining away all the information about the fluid molecules.

$$d\vec{X} = - \frac{\vec{\nabla} \bar{\Phi}(\vec{X})}{\gamma} dt + \sqrt{2\eta} d\vec{W}(t)$$

↑
effective averaged potential; free energy

What is the small parameter? Two have been considered, with different results

$$\frac{m}{M} \ll 1 \quad (\text{fluid molecule mass much smaller than solvent particle mass})$$

Under this assumption alone, the Langevin equation isn't actually correct! It turns out that you see some memory effects. Rigorously, you get an equation that looks like:

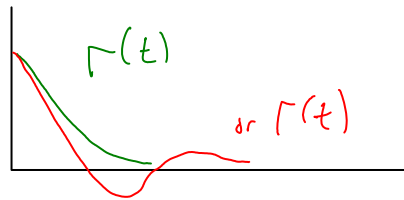
$$d\vec{X} = \vec{V} dt$$

$$M d\vec{V} = - \frac{1}{3k_B T} \left( \int_0^t \Gamma(t-s) \vec{V}(s) ds \right) dt + \sqrt{\frac{2k_B T M}{\zeta}} \int_0^t K(t-s) d\vec{W}(s)$$

$$+ \sqrt{\frac{2k_B T M}{3}} \int_0^t k(t-s) d\vec{W}(s)$$

Where  $k k^T = \Gamma$

this is Langevin equation with frictional memory given by a memory kernel of the following typical structure



Normal Langevin equation:  $\Gamma(t) = \delta(t)$

The memory arises from hydrodynamic effects. For our purposes, the main point of interest is that the stochastic noise term has a structure which again is directly connected to the friction term in a way that generalizes the relationship we had before:

$$m \frac{d\vec{V}}{dt} = -\gamma \vec{V} + g d\vec{W}(t)$$

$$g = \sqrt{2\gamma k_B T m}$$

This is no accident -- it's a consequence of a general **Fluctuation-Dissipation Theorem** which says that when thermal noise is added to a deterministic physical system based on a Hamiltonian with some added dissipation, then the noise term will be tied to the structure of the friction. Unfortunately the general discussions are rather difficult to understand, though it's not too hard to derive in any particular system by simply applying the same principles we did before -- demand consistency of the dynamics with known behavior in thermal equilibrium.

References on fluctuation-dissipation theorem:

- Kubo, "The Fluctuation-Dissipation Theorem": about the best explanation from a physically intuitive standpoint (but still very difficult to read)
- Fox and Uhlenbeck, "Contributions to Non-Equilibrium Thermodynamics. I. Theory of Hydrodynamical Fluctuations": explain how practically to apply fluctuation-dissipation relationship to derive the strength of thermal forcing in any given physical system.

It turns out that to derive the standard Langevin equation (w/o memory) from the deterministic Hamiltonian system of fluid particles and solvent particle, one not only has to assume that the mass ratio is small, but also that the density of the solute particle has to be much larger than the density of the fluid. However, it turns out that one can show Smoluchowski equation is still true without this density ratio assumption.

- References: Deutch and Oppenheim, "The Concept of Brownian Motion in Modern Statistical Mechanics"  
Bocquet, "From a Stochastic to a Microscopic Approach to Brownian Motion"