

Stochastic Mode Reduction: Klein-Kramers to Smoluchowski

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Homework 3 posted, due Friday, April 10.

We begin by nondimensionalizing the Klein-Kramers problem in terms of suitable length and time scales.

Nondimensionalization can be done as a purely formal procedure which is guaranteed to give mathematically correct transformations. However, it turns out that if one wants to pursue a perturbation theory (exploiting some small or large nondimensional parameter in the problem), then the way in which the nondimensionalization is done is actually important. Usually there is one (maybe more) good ways to nondimensionalize so that the perturbation theory can be done without complication. If one nondimensionalizes correctly but not in one of these "good" ways, then it can be difficult to formulate a reasonable perturbation theory.

If you read in books on perturbation theory about "nondimensionalizing intelligently," this is often discussed under the name "scaling" or "normalization."

The nondimensionalization procedure is to choose reference scales for all the dimensions in the problem that are naturally associated with the governing parameters (and sometimes the variables). An intelligent choice to set up perturbation theory is, when possible, to choose the choice of scales to be present in the limiting problem under consideration. Here our intuition will be that friction will be relatively strong and mass will be relatively small. ($\gamma t/m \rightarrow \infty$ was the right limit)

in force-free case; expect something similar in the presence of force.)

Guided by this intuition, we choose our reference length scale to be

$$l_F$$

because the force function still appears in the simplified problem, and it's natural to think that the length scale of the force will play an important role in determining the coarse-grained dynamics.

We also form a time scale based on parameters that still appear in the limiting problem:

$$k_B T, \gamma, l_F$$

$$\tau = \frac{l_F^2 \gamma}{k_B T}$$

This can be obtained in a few ways. Blind dimensional analysis: find exponents

$$\begin{aligned}
 J = [T] &= [l_F]^{\alpha_1} [\gamma]^{\alpha_2} [k_B T]^{\alpha_3} \\
 J &= L^{\alpha_1} (m J^{-1})^{\alpha_2} (m L^2 J^{-2})^{\alpha_3} \\
 m^0 L^0 J^1 &= m^{\alpha_2 + \alpha_3} L^{\alpha_1 + 2\alpha_3} J^{-\alpha_2 - 2\alpha_3} \\
 0 &= \alpha_2 + \alpha_3 \\
 0 &= \alpha_1 + 2\alpha_3 \\
 1 &= -\alpha_2 - 2\alpha_3 \\
 \text{Solution: } &\alpha_1 = 2, \alpha_2 = 1, \alpha_3 = -1 \\
 T &= l_F^{\alpha_1} \gamma^{\alpha_2} (k_B T)^{\alpha_3} = \frac{l_F^2 \gamma}{k_B T}
 \end{aligned}$$

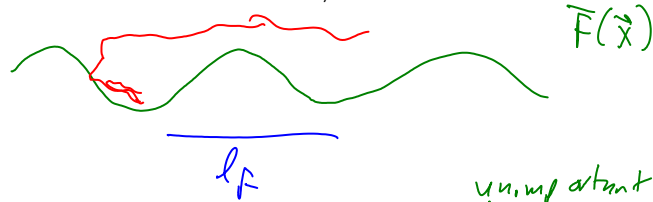
General rule of dimensional analysis is that in choosing how to combine parameters to give a desired dimension, the number of parameters involved need not be more than the number of independent dimensions in the problem, and if the number of parameters involved does not exceed the number of independent dimensions in the problem, then a power law combination will work. (One gets a singularity if the parameters don't have enough independence in their dimensions -- if this is the case choose a different set of parameters to combine.)

Or, the way I actually chose this time scale is to use physical intuition:

In the limiting problem, we expect to see the force field remain as well as the diffusivity of the particle

$$D = \frac{k_B T}{\gamma}$$

This determines a natural time scale by asking, how long would it take for the particle to diffuse over the forcing length scale (without taking into account the effect of the force on the diffusion).



This time scale $\approx \frac{l_F^2}{2D}$ because recall $D = \lim_{t \rightarrow \infty} \frac{\text{Cov}(\vec{x}(t), \vec{x}(t))}{2t}$

unimportant to keep pure numerals in reference scales mean-square displacement

$$\frac{l_F^2}{D} = \frac{l_F^2}{k_B T / \gamma} = \frac{\gamma l_F^2}{k_B T} \equiv \tau$$

We will then define nondimensional space and time variables:

$$\vec{x}' = \frac{\vec{x}}{l_F} \quad t' = \frac{t}{\tau}$$

Note that the nondimensional variables measure space and time not with respect to some artificial unit of measure (m, s). A good choice of length scales means that the nondimensional variables will vary over order unity amounts and this is good for perturbation theory.

Now, one could go ahead and nondimensionalize the velocity variable (which is another independent variable in the system) with respect to these same length and time scales:

$$\vec{v}' = \vec{v} / (l_F / \tau)$$

This would give a technically correct nondimensionalization but it turns out to be a bad idea for setting up the perturbation theory to follow. The reason this is not a good choice is because the typical size of the velocity is not l_F / τ

Instead, if we think about thermal equilibrium, then the probability distribution for the position and velocity is

$$P_{\vec{x}, \vec{v}}^{(e)}(\vec{x}, \vec{v}) = \frac{e^{-E(\vec{x}, \vec{v}) / k_B T}}{\mathcal{Z}}$$

$$= \frac{e^{-\left(\frac{1}{2} m |\vec{v}|^2 - \phi(\vec{x})\right) / k_B T}}{\mathcal{Z}}$$

if potential

Marginal distributions

$$P_{\vec{x}}^{(s)}(\vec{v}) = \int P_{\vec{x}, \vec{v}}(\vec{x}, \vec{v}) d\vec{x}$$

$$= \frac{e^{-\frac{1}{2}m|\vec{v}|^2/k_B T}}{\sqrt{2\pi k_B T/m}} \quad \text{Gaussian}$$

$$\Rightarrow \langle \vec{v} \rangle = 0$$

$$\sigma_{v_i}^2 = \frac{k_B T}{m} = \langle v_i^2 \rangle$$

$$(\text{cov}(\vec{v}, \vec{v})) = \frac{k_B T}{m} \mathbf{1}$$

This suggests that a better choice of velocity scale is

$$v = \sqrt{\frac{k_B T}{m}}$$

$$\vec{v}' = \frac{\vec{v}}{v} = \frac{\vec{v}}{\sqrt{k_B T/m}}$$

only appears in detailed problem but ok because \vec{v} doesn't appear in simplified problem

What's good about this is that the nondimensionalized velocity variable will take typical order unity values.

We have now chosen nondimensional independent variables; we must also nondimensionalize the dependent variable, which is the PDF:

$$[P_{\vec{x}, \vec{v}}] = \ell^{-d} (\ell/J)^{-d} \quad \text{in } d \text{ dimensions}$$

$$P(\vec{x} \in A, \vec{v} \in B) = \int_A d\vec{x} \int_B d\vec{v} P_{\vec{x}, \vec{v}}(\vec{x}, \vec{v})$$

\uparrow \uparrow \uparrow
 $n \text{ dimensions}$ $\dim \Sigma^d$ $\dim (\Sigma/J)^d$

Since this PDF refers directly to the properties of the variables \vec{x} and \vec{v} , we naturally use those scales to nondimensionalize the PDF

$$P'_{\vec{x}, \vec{v}}(\vec{x}', \vec{v}') = \frac{P_{\vec{x}, \vec{v}}(\vec{x}' \ell_P, \vec{v}' \frac{\sqrt{k_B T}}{m})}{\ell_P^{-d} \left(\frac{\sqrt{k_B T}}{m}\right)^{-d}}$$

Now we've defined the transformation, now we arrive at the purely mechanical task of changing variables from dimensional to nondimensional variables. Basically just use chain rule over and over in a trivial way.

$$\left(\frac{\partial P_{\vec{x}, \vec{v}}(\vec{x}, \vec{v})}{\partial t} \right) = \left(\frac{dt'}{dt} \right) \frac{\partial}{\partial t'} \left(P'_{\vec{x}, \vec{v}}(\vec{x}', \vec{v}') \ell_P^{-d} \left(\frac{\sqrt{k_B T}}{m} \right)^{-d} \right)$$

$\frac{dt'}{dt} = k_B T / \ell_P^2 \gamma$

Basically just use chain rule over and over in a trivial way.

$$\frac{\partial p_{\vec{x}, \vec{v}}(\vec{x}, \vec{v})}{\partial t} = \frac{dt'}{dt} \frac{\partial}{\partial t'} \left(p'_{\vec{x}, \vec{v}}(\vec{x}', \vec{v}') l_F^{-d} \left(\sqrt{\frac{k_B T}{m}} \right)^d \right)$$

dimensional

Chain rule is simple because

$$t' = g_1(t)$$

$$\vec{x}' = g_2(\vec{x})$$

$$\vec{v}' = g_3(\vec{v})$$

nondimensional

$$= \left(\frac{k_B T}{l_P^2 \gamma} \right) \left(l_P^{-d} \left(\sqrt{\frac{k_B T}{m}} \right)^{-d} \right) \frac{\partial p'_{\vec{x}, \vec{v}}(\vec{x}', \vec{v}')}{\partial t'}$$

We proceed in this way, using the chain rule to write:

$$\vec{\nabla}_{\vec{x}} = \left(\vec{\nabla}_{\vec{x}'} \vec{x}' \right)^T \cdot \vec{\nabla}_{\vec{x}'} = \left(l_P^{-1} \right)^T \cdot \vec{\nabla}_{\vec{x}'} = \frac{1}{l_P} \vec{\nabla}_{\vec{x}'}$$

dimensional

Jacobian $\vec{x} \rightarrow \vec{x}'$

$$\vec{\nabla}_{\vec{v}} = \frac{1}{\sqrt{\frac{k_B T}{m}}} \vec{\nabla}_{\vec{v}'}$$

nondimensional

$$\Delta_{\vec{v}} = \vec{\nabla}_{\vec{v}} \cdot \vec{\nabla}_{\vec{v}} = \left(\frac{1}{\sqrt{\frac{k_B T}{m}}} \right)^2 \vec{\nabla}_{\vec{v}'} \cdot \vec{\nabla}_{\vec{v}'} = \frac{1}{\frac{k_B T}{m}} \Delta_{\vec{v}'}$$

LWS at Klein-Kramers:

$$\left(\frac{k_B T}{l_P^2 \gamma} \right) \left(l_P^{-d} \left(\sqrt{\frac{k_B T}{m}} \right)^{-d} \right) \frac{\partial p_{\vec{x}, \vec{v}}}{\partial t'}$$

RHS at Klein-Kramers:

$$= -\frac{1}{l_P} \vec{\nabla}_{\vec{x}'} \cdot \left(\vec{v}' \sqrt{\frac{k_B T}{m}} \right) p'_{\vec{x}, \vec{v}} \left(l_P^{-d} \left(\sqrt{\frac{k_B T}{m}} \right)^{-d} \right)$$

$$+ \frac{1}{\sqrt{\frac{k_B T}{m}}} \vec{\nabla}_{\vec{v}'} \cdot \left(\left(\frac{\gamma \vec{v}' \sqrt{\frac{k_B T}{m}}}{m} - \frac{\vec{F} f(\vec{x}')}{m} \right) p'_{\vec{x}, \vec{v}} \left(l_P^{-d} \left(\sqrt{\frac{k_B T}{m}} \right)^{-d} \right) \right)$$

$$+ \frac{\gamma k_B T}{m^2} \left(\frac{1}{k_B T} \right) \Delta_{\vec{v}'} \left(p'_{\vec{x}, \vec{v}} \left(l_P^{-d} \left(\sqrt{\frac{k_B T}{m}} \right)^{-d} \right) \right)$$

$\vec{F}(\vec{x}) = \vec{F} f(\vec{x}'/l_P)$

$$+ \frac{1}{\sqrt{\frac{k_B T}{m}}} \nabla_{v'} \cdot \left(\left(\frac{\gamma \vec{v}' \sqrt{\frac{k_B T}{m}}}{m} - \frac{\vec{F} f(\vec{x}')}{m} \right) P_{\Sigma, \Sigma} (l_F^{-d}) \left(\sqrt{\frac{k_B T}{m}} \right)^{-d} \right)$$

$$+ \frac{\gamma k_B T}{m^2} \left(\frac{1}{\frac{k_B T}{m}} \right) A_{v'} \left(P_{\Sigma, \Sigma} (l_F^{-d}) \left(\sqrt{\frac{k_B T}{m}} \right)^{-d} \right)$$

Cancel some obvious common factors (with the red arrow) then multiply both sides by $\frac{l_F^2 \gamma}{k_B T}$

dimensional

$$\frac{\partial p'_{\Sigma, \Sigma}}{\partial t'} = - \frac{l_F \gamma}{\sqrt{k_B T m}} \nabla_{x'} \cdot (\vec{v}' P_{\Sigma, \Sigma})$$

$$+ \nabla_{v'} \cdot \left(\left(\frac{l_F^2 \gamma^2}{k_B T m} \vec{v}' - \frac{l_F^2 \gamma \vec{F} f(\vec{x}')}{(k_B T)^{3/2} m^{1/2}} \right) P_{\Sigma, \Sigma} \right)$$

$$+ \frac{l_F^2 \gamma^2}{k_B T m} A_{v'} P_{\Sigma, \Sigma}$$

Now the goal is to identify nondimensional parameters. This can be done mechanically but it will be better to do so with some thought. Mechanically speaking, we started with 5 parameters and 3 variables, and we have three independent dimensions (mass, length, and time), which mean we are guaranteed (by something called Buckingham-Pi theorem in dimensional analysis) that the problem can be formulated in terms of 5-3=2 nondimensional parameters and 3 nondimensional variables. One can just construct arbitrary choices for the 2 nondimensional parameters, but it's best to let the equation guide the choice, using dimensional consistency.

Let's choose two good nondimensional parameters in terms of which the nondimensional equation takes a good form.

$$\epsilon = \frac{\sqrt{k_B T m}}{l_F \gamma}$$

$$\mu = \frac{l_F^2 \gamma \bar{F}}{(k_B T)^{3/2} m^{1/2}} \quad \epsilon = \frac{l_F \bar{F}}{k_B T}$$

doesn't involve any parameter disappearing in simplification

Why this choice for the second nondimensional parameter? We're preparing to set up a perturbation theory where we will want to take the limit in which one nondimensional parameter becomes small or large, and it's easiest if the other nondimensional parameters in the problem can be held fixed in this limit. (It's very difficult and usually not possible to do perturbation theory with multiple small and large parameters unless they are linked together in a distinguished limit.)

Our nondimensionalized Klein-Kramers equation then reads:

$$\frac{\partial p'}{\partial t'} = - \epsilon^{-1} \nabla_{x'} \cdot (\vec{v}' p')$$

$$+ \epsilon^{-2} \nabla_{v'} \cdot (\vec{v}' p')$$

$$- \epsilon^{-1} \mu \nabla_{v'} \cdot (\vec{F}(\vec{x}') p')$$

$$t \quad \epsilon^{-2} \Delta_{V'} p'$$

This equation is rigorously equivalent to the original equation in that any solution to this equation is associated to a solution of the original PDE by just inverting the change of variables. Note that this equation just has 2 parameters and 3 variables, rather than 5 parameters and 3 variables in the original equation.