Multiscale Computing and Escape Problems

Friday, April 17, 2009
12:02 PM

$$d\vec{X} = \vec{a}(\vec{X}, \vec{Y})\, dt \qquad \text{slow}$$

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

fast

Some applications where this numerical multiscale approach has been deployed (when extended to PDE's):

- "superparameterization" in atmosphere weather/climate modeling
- CONFESSIT by Öttinger for simulating complex fluids

$$\rho\left(\frac{\partial \vec{u}}{\partial t} + \vec{u}\cdot\vec{\nabla}\vec{u}\right) = -\vec{\nabla}\cdot S$$

mass density — fluid velocity — stress tensor

For simple fluids $\quad S = p\, I - \eta\left(\vec{\nabla}\vec{u} + \vec{\nabla}\vec{u}^{T}\right)$

pressure — dynamic viscosity

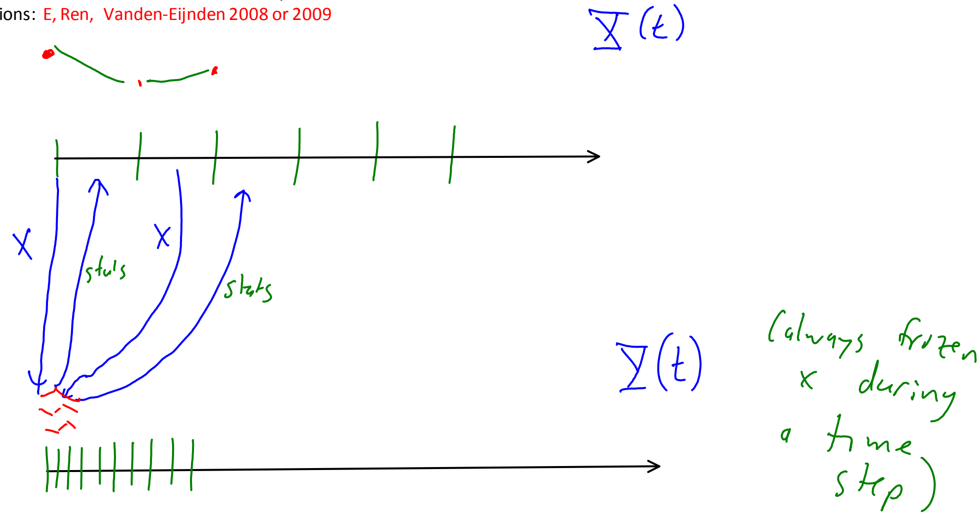
For more complex fluids, the stress tensor is not so easy to describe in terms of the large scale fluid velocity. The stress tensor also involves the configuration of the immersed structures and their material properties.

The multiscale approach works like this: The stress tensor has a rigorous definition in terms of the statistics of the small-scale structures. But the time scale on which the small immersed structures evolve is fast compared to the large-scale fluid flow in which one is interested. Simulating the immersed structures and the fluid would create a stiff system.

In the multiscale approach, one effectively simulates the fast microstructures over a short time period, takes their statistics, uses it to compute the stress tensor, then take a large time step for the fluid variables. Repeat the procedure.

Material science application to crack propagation

Very recent innovation on multiscale techniques which makes more seamless simulations: E, Ren, Vanden-Eijnden 2008 or 2009



This seamless approach was motivated by a relatively old idea by Car-Pirinello for molecular dynamics computations. The basic idea is that if the time scale separation ε is small enough, then its value doesn't affect the dynamics of the slow variables interest. So since a small ε makes the systems stiff, choose ε to be not so small.

Homework 3 due on Tuesday, April 21 at noon.

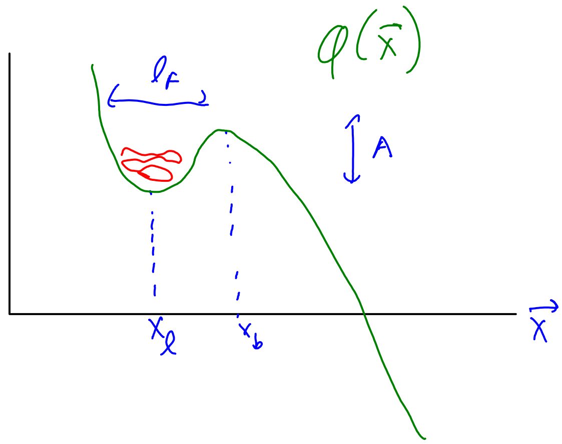
Rate of Diffusion of a Particle over a Barrier (Kramers problem)

neglect inertia

Solve for

$$\cancel{m\, d\vec{V}} = -\gamma \vec{V}\, dt + \sqrt{2 k_B T \gamma}\, d\vec{W}(t) - \vec{\nabla}\varphi(\vec{X})\, dt$$

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



The basic question is how long does it take for the particle to escape the local minimum by passing over the barrier. This is most interesting when thermal fluctuations are needed for this to happen.

We'll treat this just as a physical problem but its solution has applications to many areas:

- chemical kinetics (molecular disassociation, nuclear reactions, configurational changes): the variable x is like a reaction coordinate (more recent work: "commitor variable")
- coagulation of sediment
- diffusion in solids and electronic transport

We will work only with the overdamped case simply because it's easier. Without this assumption, many calculations can still be done, but with much more labor. (Risken, Fokker-Planck Equation, Ch. 11)

Overdamped case: friction formally dominates mass and therefore inertia is neglected.

$$d\vec{X} = -\frac{1}{\gamma}\vec{\nabla}\phi(\vec{X})\, dt + \sqrt{2D}\, d\vec{W}(t)$$

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

Reference: Risken Sec. 5.10

This problem is most interesting when the thermal energy is weak compared to the barrier height, so that one must wait a long time to see the barrier crossed. This sounds like asymptotics so let's do this properly.

First we nondimensionalize:

Let's write the structure of the dimensional potential as:

$$\varphi(\vec{x}) = A\, \hat{\varphi}\left(\frac{\vec{x}}{\ell_F}\right)$$

nondimensional potential

Parameters: $[\ell_F] = \mathcal{L}$
$[A] = \mathcal{M}\mathcal{L}^2\mathcal{T}^{-2}$
$[k_B T] = \mathcal{M}\mathcal{L}^2\mathcal{T}^{-2}$
$[\gamma] = \mathcal{M}\mathcal{T}^{-1}$

Length scale ℓ_F

Length scale l_F

Time scale? $\tau = l_F^{\alpha_1} A^{\alpha_2} \gamma^{\alpha_3}$

(leave out $k_B T$ which should be weak)

$$[\tau] = [l_F]^{\alpha_1} [A]^{\alpha_2} [\gamma]^{\alpha_3}$$

$$\tau = \frac{\gamma l_F^2}{A}$$

This scales with the time it takes for particle to fall from top of barrier to bottom of local minimum:

Force $\sim \frac{A}{l_F}$

Velocity $\sim \frac{\text{Force}}{\gamma} \sim \frac{A/l_F}{\gamma} = \frac{A}{l_F \gamma}$

Time $\sim \frac{\text{Length}}{\text{Velocity}} \sim \frac{l_F}{A/l_F\gamma} = \frac{\gamma l_F^2}{A} = \tau$

$$x' = \frac{x}{l_F} \qquad t' = \frac{t}{\tau} = \frac{A t}{\gamma l_F^2}$$

And, as is usually (but not always) the case, it's easier to do asymptotics on the deterministic Fokker -Planck equation than on the SDE's. We'll just do one-dimensional case, which is actually of wide importance, though higher dimensions can also be done.

$$\frac{\partial p(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(\frac{1}{\gamma}\frac{d\Phi}{dx}\, p(x,t)\right) + \frac{\partial^2}{\partial x^2}\Big(D\, p(x,t)\Big)$$

Nondimensionalize the probability density

$$p(x,t) = \frac{1}{l_F}\, p'\Big(\underbrace{\frac{x}{l_F}}_{=x'}, \underbrace{\frac{t}{\tau}}_{=t'}\Big)$$

Plug into equation, chain rule to change to new variables

$$\frac{\partial p}{\partial t} = \frac{dt'}{dt}\frac{\partial}{\partial t'}\left(\frac{1}{l_F}\, p'(x',t')\right) = \frac{1}{\tau}\frac{1}{l_F}\frac{\partial p'(x',t')}{\partial t'}$$

$$\frac{\partial}{\partial x}\left(\frac{1}{\gamma}\frac{d\varphi}{dx}\,p(x,t)\right)+\frac{\partial^2}{\partial x^2}\Big(D\,p(x,t)\Big)$$

$$=\underbrace{\frac{dx'}{dx}}_{=\frac{1}{l_p}}\frac{\partial}{\partial x'}\left(\frac{1}{\gamma}\frac{dx'}{dx}\frac{d}{dx'}\Big(A\,\hat{\varphi}(x')\Big)\frac{1}{l_p}\,p'(x',t')\right)$$

$$+\left(\frac{dx'}{dx}\right)^2\frac{\partial^2}{\partial x'^2}\left(D\,\frac{1}{l_p}\,p'(x',t')\right)$$

$$=\frac{A}{l_p^3\,\gamma}\frac{\partial}{\partial x'}\left(\frac{d\hat{\varphi}}{dx'}\,p'(x',t')\right)+\frac{D}{l_p^3}\frac{\partial^2 p'(x',t')}{\partial x'^2}$$

Equating LHS = RHS, multiply $\times\, T\, l_p$

$$\frac{\partial p'(x',t')}{\partial t'}=\underbrace{\frac{AT}{l_p^2\,\gamma}}_{=1}\frac{\partial}{\partial x'}\left(\frac{d\hat{\varphi}}{dx'}\,p'(x',t')\right)+\underbrace{\frac{TD}{l_p^2}}_{=\frac{D\gamma}{A}=\frac{k_B T}{A}\equiv\varepsilon}\frac{\partial^2 p'(x',t')}{\partial x'^2}$$

$$T=\gamma\, l_p^2/A$$