Stochastic Advection-Diffusion equations

By considering simple models of diffusion we obtained the stochastic diffusion equation SPDE

$$\partial_t \rho = \nabla \cdot \left\{ D \nabla \rho + \sqrt{2 m D \rho}\, \mathcal{W}(r, t) \right\}$$

The first step is to understand what this equation really means and how to solve it at equilibrium or some simple non-equilibrium settings.

The nonlinear SPDE as written is hard to analyse and may even be ill-defined. In particular, there does not appear to be a well-defined way to interpret the meaning of non-linear functionals of white noise or products of distributions.

By contrast, the case of linear SPDEs is easy and lots can be done analytically.

Recall that fluctuations scale like

$$1/\sqrt{N_s} \leftarrow \text{coarsening scale}$$

We will assume that fluctuations are small and we can linearize the SPDEs around a steady or equilibrium state:

$$\boxed{\rho = \bar{\rho} + \delta\rho}\quad , \quad \bar{\rho} \equiv \bar{\rho}(r)$$

At equilibrium though $\bar{\rho} = \rho_0 = \text{const.}$

As will become clear shortly, when linearizing the stochastic flux only the zeroth-order (no $\delta\rho$) terms need to be retained.

$$\partial_t (\delta\rho) = \nabla \cdot \left\{ D \nabla (\delta\rho) + \sqrt{2mD\rho_0}\; \mathcal{W}(r,t) \right\}$$

$\Downarrow$ simplify notation $(\delta\rho) \to \rho$

reserve D for later

$$\boxed{\partial_t \rho = \nabla \cdot \left\{ \chi \nabla \rho + (2\chi S)^{1/2} \cdot \mathcal{W}(r,t) \right\}}$$

constant

How do we now solve or analyse this SPDE?

Answer: In Fourier space:

$$\rho \to \hat{\rho}(k)$$

wave number

$$\partial_t \rho = \chi \nabla^2 \rho + \sqrt{2 S \chi}\,(\nabla \cdot \mathcal{W})$$

$$\partial_t \hat{\rho} = -\chi k^2 \hat{\rho} + \sqrt{2 S \chi}\,(i k \hat{\mathcal{W}}) \leftarrow \text{SODE!}$$

What does spatial white noise look like in Fourier-space?

$\hat{\mathcal{W}}(k; t)$ is white-noise (in t) independent of other k's

$$\boxed{\langle \hat{\mathcal{W}}(k_1, t_1)\, \hat{\mathcal{W}}^*(k_2, t_2) \rangle = \delta(k_1 - k_2)\, \delta(t_1 - t_2)}$$

So we have one SODE per wavenumber ... now it is easy.

$$\partial_t \hat{\rho} = -\chi k^2 \hat{\rho} + \sqrt{2S\chi} \cdot ik\, \hat{W}$$

This is a Langevin equation

($\hat{\rho}$ like velocity)

Compare to what we had for Langevin:

$$\begin{cases} \dot{v} = -\frac{\gamma}{m} v + \sqrt{2\gamma (k_B T)}\, W(t) \\ \Downarrow \quad \langle v^2 \rangle = k_B T / m \\ P(v) = Z^{-1} e^{-mv^2/2k_B T} \end{cases}$$

$\Rightarrow$ correspondence $\begin{cases} \gamma \Leftrightarrow \chi k^2 \\ S \Leftrightarrow k_B T \end{cases}$

The variance of $\hat{\rho}(k)$ is thus:

$$\boxed{\langle \hat{\rho}\hat{\rho}^* \rangle = S = m\rho}$$

independent of k (WHITE NOISE)

we will derive this again later

More specifically, since different wavenumbers are uncorrelated,

$$\boxed{\langle \hat{\rho}(k)\, \hat{\rho}^*(k') \rangle = m\rho\, \delta(k-k')}$$

which means that a typical snapshot of ρ looks like spatial <u>white-noise</u>.

The quantity

$$S(k) = \langle \hat{\rho}(k) \hat{\rho}^*(k) \rangle$$

is called the <u>static structure factor</u> in physics.

What does it imply in real space:

$$\rho(\vec{r}) = (\text{normalization}) \int \hat{\rho}(\vec{k})\, d\vec{k} \cdot e^{i\vec{k}\cdot\vec{r}}$$

Consider now the <u>average density</u> inside a box of length Δx, volume

$$\Delta V = \Delta x^d$$

$$\rho_{\Delta V} = \frac{1}{\Delta V} \int_{\Delta V} \rho(r)\, dr \Rightarrow$$

$$\langle \rho_{\Delta V} \rho^*_{\Delta V'} \rangle = \frac{1}{\Delta V^2} \left\langle \int_{\Delta V} \int_{\Delta V'} \rho(r) \rho^*(r')\, dr\, dr' \right\rangle$$

two different hydrodynamic cells

$$= \frac{1}{\Delta V^2} \int_{\Delta V} dr \int_{\Delta V'} dr' \int_k dk \int_{k'} dk' \cdot e^{i(kr - k'r')} \langle \hat{\rho}(k) \hat{\rho}^*(k') \rangle$$

but recall

$$S(k)\, \delta(k - k')$$

$$\left\{ \langle \rho_{\Delta V} \rho^{*}_{\Delta V'} \rangle = \frac{1}{\Delta V^2} \int_{\Delta V} dr \int_{\Delta V'} dr' \int dk \cdot e^{ik\cdot(r-r')} \cdot \underset{\substack{\parallel \\ S = \text{const.}}}{S(k)} \right.$$

Due to orthonormality of the Fourier basis, the integral over k gives $\delta(r-r')$, or

$$\langle \rho_{\Delta V} \rho^{*}_{\Delta V'} \rangle = \frac{S}{\Delta V^2} \int_{\Delta V} dr \int_{\Delta V'} dr' \; \delta(r-r')$$

$$\boxed{\langle \rho_{\Delta V}\, \rho^{*}_{\Delta V'} \rangle = \begin{cases} \dfrac{S}{\Delta V} & \text{if } \Delta V \equiv \Delta V' \\ 0 & \text{otherwise} \end{cases}}$$

Fluctuations in distinct hydrodynamic cells at equilibrium are uncorrelated, and the variance of $\rho_{\Delta V}$ is:

$$\langle \delta\rho_{\Delta V}^{2} \rangle = \frac{S}{\Delta V} = \frac{m\rho_0}{\Delta V} = \frac{m \cdot \left(\dfrac{m\bar{N}_p}{\Delta V}\right)}{\Delta V}$$

$$\langle \delta\rho_{\Delta V}^{2} \rangle = \frac{m^2}{\Delta V^2} \cdot \bar{N}_p \quad \text{since } \boxed{\langle \delta N_p^2 \rangle = \bar{N}_p}$$

Poisson!

So far we were sloppy with normalization factors for the Fourier transforms.
There are different definitions with factors of (2π) placed either in $\exp(2\pi i \xi r)$, or as $\frac{1}{(2\pi)^d}$ or $\frac{1}{(2\pi)^{d/2}}$ prefactors.
As long as a consistent definition is used and the appropriate (2π) is considered in $\langle \hat{W}(k_1) W^*(k_2) \rangle$ it is OK.

Best is to consider a finite periodic system and use a Fourier series instead of an integral:

$$\begin{cases} \rho(r) = \sum\limits_{k = \frac{2\pi \kappa}{L},\ \kappa \in \mathbb{Z}^d} e^{ik\cdot r}\,\hat{\rho}(k) \\ \hat{\rho}(k) = \frac{1}{L^d} \int e^{-ik\cdot r}\,\rho(r)\,dr \end{cases}$$

Analogous definitions exist in the discrete setting, $\frac{1}{L^d} \Leftrightarrow \frac{1}{N_c}$

Consider white noise $W(r)$:

$$\langle \hat{W}(k)\, \hat{W}^*(k') \rangle = \frac{1}{L^2} \int_r \int_{r'} e^{i(k'r' - kr)} \, dr\, dr' \, \langle W(r) W^*(r') \rangle$$

1D for now

this is $\delta(r-r')$

$$= \frac{1}{L^2} \int_{r=0}^{L} dr \; e^{i(k'-k)\cdot r} = \frac{1}{L^2} \cdot L \cdot \delta_{KK'}$$

$$\boxed{\langle \hat{W}(k)\, \hat{W}^*(k') \rangle = \frac{1}{V} \delta_{KK'}}$$

system volume

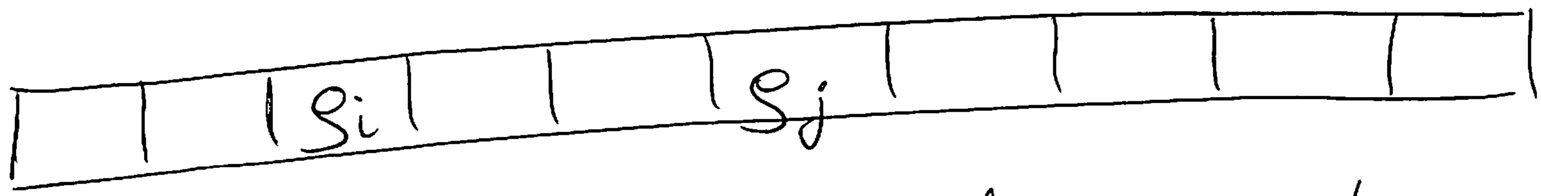
This calculation shows that in any orthonormal basis the <u>weights</u> (coefficients) of white noise are i.i.d Gaussian random variables with mean zero and variance unity. This is in fact the way to give rigorous meaning to <u>cylindrical Brownian motion</u> or <u>Brownian sheets</u> and the SPDEs (at least linearized). In the <u>non-linear</u> setting truncation changes the SPDE, however.

Discretizing the volume into N_c cells of volume $\Delta V = \frac{V}{N_c}$ is closely-related to <u>truncating Fourier space</u> representations to the first N_c modes (wavenumbers).

By Parseval's theorem, the variance in real space is

$$\langle W_{\Delta V} W^*_{\Delta V'} \rangle = \langle W^2_{\Delta V} \rangle \delta_{\Delta V, \Delta V'}$$

$$\langle W^2_{\Delta V} \rangle = N_c \langle \hat{W} \cdot \hat{W}^* \rangle = \frac{1}{\Delta V} \leftarrow \text{as before}$$



We can thus judge how good a discretization is by examining the discrete structure factor at equilibrium

$$S(k) = V \langle \hat{\rho}(k) \hat{\rho}^*(k) \rangle = 1 \quad \text{(ideally)}$$

independent of wavenumber

discrete spectrum

which implies the correct covariance in real space

$$\boxed{\langle (\delta\rho_i)(\delta\rho_j) \rangle = \frac{m \rho_0}{\Delta V} \delta_{ij}}$$

When discretizing white noise, what we are doing is truncating the spectrum at wavenumber $k_{max} = \frac{\pi}{\Delta x}$, or equivalently, representing $\mathcal{W}(r,t)$ with its space-time <u>finite-volume</u> average

$$\frac{1}{\Delta x \, \Delta t} \iint_{t = n\Delta t,\, r \in \Delta V_i}^{(n+1)\Delta t} \mathcal{W}(r,t)\, dr\, dt \iff \frac{\widetilde{\mathcal{W}}_i^n}{\sqrt{\Delta x \cdot \Delta t}}$$

where $\widetilde{\mathcal{W}}_i$ is a normally-distributed (Gaussian) unit random variate.

The continuum SPDE

$$\begin{cases} \partial_t u = \chi \nabla^2 u + \sqrt{2\chi S} \cdot (\nabla \cdot \mathcal{W}) \\ \quad\;\; = L u + K \mathcal{W} \end{cases}$$

where $\begin{cases} L \equiv \chi \nabla^2 \\ K = \sqrt{2\chi S}\ \nabla \cdot \end{cases}$ are linear differential operators

Or, in Fourier space

$$\begin{cases} \partial_t \hat{u} = -\chi k^2 \hat{u} + \sqrt{2S\chi}\ (ik)\,\hat{\mathcal{W}} \\ \quad\;\; = \hat{L}\,\hat{u} + \hat{K}\,\hat{\mathcal{W}} \end{cases}$$

A spatial discretization of this stochastic diffusion equation would have the form

$$\partial_t \vec{u} = L\vec{u} + K\widetilde{W}$$

where L is now a <u>discrete Laplacian</u>,

e.g.

$$(L\vec{u})_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}$$

and K is a <u>discrete divergence</u>, e.g.

$$(K\widetilde{W})_i = \frac{\widetilde{W}_{i+1} - \widetilde{W}_{i-1}}{2\Delta x} \leftarrow \text{Sandra's talk}$$

For periodic boundary conditions, we can use a discrete Fourier transform to translate to

$$\partial_t \hat{\vec{u}} = \hat{L}\,\hat{\vec{u}} + \hat{K}\,\hat{\vec{W}}$$

"symbols" of L and K

e.g.
$$\begin{cases} \hat{L} = \dfrac{e^{ik\Delta x} - 2 + e^{-ik\Delta x}}{\Delta x^2} \\[2ex] \hat{K} = \dfrac{e^{ik\Delta x} - e^{-ik\Delta x}}{2\Delta x} \end{cases}$$

In all cases, discrete or continuous, or real space or Fourier space, we have a simple SDE with additive noise:

$$\partial_t u = L u + K W$$

So let's analyze this in more detail, for general linear operators L and K.

The basic property at equilibrium is the <u>steady-state covariance</u>

$$C = \langle u u^* \rangle$$ ← equilibrium ensemble (or time average by ergodicity argument)

First approach is to look at the function:

$$C(u(r,t)) = c(u) = u u^*$$

and use Ito's formula or the Backward Kolmogorov equation

$$\partial_t C = (Lu) \cdot \frac{\partial}{\partial u} C + \frac{1}{2} (K K^*) : \frac{\partial}{\partial u^2} C = 0$$

BVP

at steady state

Let's switch to indicial notation to figure out the contractions:

$$\left[(Lu)\cdot\frac{\partial}{\partial u}(uu^*)\right]_{jk}=(Lu)_i\,\frac{\partial}{\partial u_i}(u_j u_k)$$

$$=L_{il}u_l\left[\delta_{ij}u_k+\delta_{ik}u_j\right]=$$

$$=L_{jl}u_l u_k+u_j u_l L^*_{lk}$$

$$=LC+CL^*$$

(Note that $C^*=C$)

Similarly, $\frac{1}{2}(KK^*) : \frac{\partial}{\partial u^2}(uu^*) = KK^*$

So we get the <u>linear system</u> or linear boundary-value problem:

$$\boxed{LC + CL^* = KK^*}$$

discrete, continuum
real or Fourier

At thermodynamic equilibrium, recall that for the simple diffusion equation $u \equiv \rho$ we have

structure factor

$$\langle uu^* \rangle = \frac{S}{\Delta V} I$$

identity

This gives the <u>fluctuation-dissipation</u> balance condition

DFDB: $$\boxed{L + L^* = \frac{\Delta V}{S} K K^*}$$

Recall

spatially discrete white noise

$$\begin{cases} \partial_t u = \chi \mathcal{L} u + \sqrt{2\chi S}\, \mathcal{D}\left(\dfrac{\mathcal{W}}{\sqrt{\Delta V}}\right) \\ \text{discrete} \quad \text{Laplacian} \quad \text{divergence} \end{cases}$$

$$\Rightarrow \quad L = \chi \mathcal{L}, \quad K = \sqrt{\frac{2\chi S}{\Delta V}}\, \mathcal{D}$$

Note DFDB is satisfied if:

$$\boxed{\mathcal{L} = \mathcal{D}\mathcal{D}^*}$$

which is analogous $\nabla^2 = \nabla \cdot \nabla$

It is not too hard to construct spatial discretizations that obey this condition, as we will discuss next time.

We can also easily include <u>advection</u> in this picture, i.e., consider the <u>stoch.</u> <u>advection-diffusion</u> equation:

$$\boxed{\partial_t \rho + v \cdot \nabla \rho = \chi \nabla^2 \rho + \sqrt{2 \varepsilon \chi}\, \nabla \cdot \mathcal{W}(r,t)}$$

where v is a specified (constant) velocity field

$$\boxed{\nabla \cdot v = 0}$$

Now $L = \chi \nabla^2 + v \cdot \nabla$

$$= \chi \mathcal{L} + \underbrace{A(v)}_{\text{advection operator}}$$

Note that $L + L^* = 2\chi\mathcal{L} = \frac{\Delta V}{S} K K^*$

and thus DFDB is not affected by advection because of the fact that

advection is skew-adjoint

$$\boxed{A^*(v) = -A(v)}$$ ← advection does not dissipate or amplify fluctuations

This follows from

$$\int_{\Omega} w\,[v\cdot\nabla c]\,dr = \int w\,\nabla\cdot[c v]\,dr$$

$$= -\int c\,\nabla\cdot[w v]\,dr = -\int c\,[v\cdot\nabla w]\,dr$$

under periodic boundary conditions or no-slip BCs:

$$\nabla\cdot v = 0 \text{ in } \partial\Omega, \quad v\cdot n_{\partial\Omega} = 0$$

Similarly, $\boxed{\nabla^{*} = -\nabla\cdot}$ since

$$\int w\,(\nabla\cdot v)\,dr = -\int v\cdot\nabla w\,dr$$

A spatio-temporal discretization could be based on the Euler scheme (really Euler-Maruyama)

$$\boxed{u^{n+1} = u^{n} + \chi \mathcal{L} u^{n} \Delta t + \sqrt{\frac{2\chi S \Delta t}{\Delta V}}\, \mathcal{D} W}$$

and the construction of appropriate discrete differential operators will be discussed next time.

Note that the stochastic forcing can be added to any deterministic scheme

$\boxed{\text{discrete white noise}} \iff \frac{1}{\sqrt{\Delta t \, \Delta V}} W$