Stochastic Advection- Diffusion equations

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

\[ \partial_t S = \nabla \cdot \left( \mathbf{D} \nabla S + \sqrt{2m} \mathbf{D} \mathbf{G} \mathbf{W}(r,t) \right) \]

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 \( \frac{1}{\sqrt{N_S}} \) coarse graining scale.
We will assume that fluctuations are small and we can linearize the SPDEs around a steady or equilibrium state:

\[ S = \bar{S} + \delta S \]

At equilibrium, though \( \bar{S} = \bar{S}_0 = \text{const.} \)

As will become clear shortly, when linearizing the stochastic flux, only the zeroth-order (no \( \delta S \)) terms need to be retained.
\[ \partial_t (\bar{g}) = \nabla \cdot \left\{ \nabla \nabla (\bar{g}) + \sqrt{2mD_0} \bar{g} \cdot W(r,t) \right\} \]

\[ \sqrt{\text{simplify notation } (\bar{g}) \rightarrow g} \]

\[ \nabla \text{ reserve } D \text{ for later } \]

How do we now solve or analyse this SPDE?

Answer: In Fourier Space:

\[ g \rightarrow \hat{g}(k) \]

\[ \text{wave number} \]
\[ \partial_t \mathcal{S} = x \nabla^2 \mathcal{S} + \sqrt{2\kappa} (\nabla \cdot \mathbf{W}) \]
\[ \partial_t \hat{\mathcal{S}} = -x k^2 \hat{\mathcal{S}} + \sqrt{2\kappa} (i k \hat{\mathbf{W}}) \leftarrow \text{SODE} ! \]

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

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

\[ \langle \hat{W}(k_1, t_1) \hat{W}(k_2, t_2) \rangle = \delta(k_1 - k_2) \delta(t_1 - t_2) \]

So we have one SODE per wavenumber ... now it is easy.
\[ \dot{\mathbf{g}} = -\chi k^2 \mathbf{g} + \sqrt{2S} \mathbf{i} k \mathbf{w} \]

This is a Langevin equation

(\hat{\mathbf{g}} \text{ like velocity})

Compare to what we had for Langevin:

\[
\begin{aligned}
\dot{\mathbf{u}} &= -\frac{\mathbf{u}}{m} \mathbf{u} + \sqrt{2 g(k_B T)} \mathbf{w}(t) \\
\downarrow &\quad \langle \mathbf{u}^2 \rangle = k_B T / m \\
P(\mathbf{u}) &= \frac{1}{\pi} - \frac{m \mathbf{u}^2}{2 k_B T} \\
\end{aligned}
\]

\[ \Rightarrow \text{correspondence} \]

\[ \mathbf{g} \leftrightarrow X k^2 \]

\[ \mathbf{s} \leftrightarrow k_B T \]
The variance of $\hat{S}(k)$ is thus:

$$\langle \hat{S} \hat{S}^* \rangle = \sigma^2 = mg$$

we will derive this again later.

More specifically, since different wave-numbers are uncorrelated,

$$\langle \hat{S}(k) \hat{S}^*(k') \rangle = mg \delta(k-k')$$

which means that a typical snapshot of $S$ looks like spatial white noise.
The quantity
\[ S(k) = \langle \hat{\xi}(k) \hat{\xi}^*(k) \rangle \]
is called the \underline{static structure factor}
in physics.
What does it imply in real space:
\[ S(\mathbf{r}) = \text{(normalization)} \int \hat{\xi}^{\mathbf{r}}(\mathbf{k}) \hat{\xi}^{\mathbf{r}}(\mathbf{k}) \, d\mathbf{k} \cdot e^{i \mathbf{k} \cdot \mathbf{r}} \]
Consider now the \underline{average density}
inside a box of length \( \Delta x \),
volume \( \Delta V = \Delta x \).
\[ S_{\Delta V} = \frac{1}{\Delta V} \int_{\Delta V} S(r) \, dr \quad \Rightarrow \]

\[
\langle S_{\Delta V} S_{\Delta V'}^* \rangle = \frac{1}{\Delta V^2} \left\langle \int \int S(r) S^*(r') \, dr \, dr' \right\rangle
\]

\[
\uparrow \quad \uparrow \quad \text{two different} \quad \text{hydrodynamic cells}
\]

\[
= \frac{1}{\Delta V^2} \int_{\Delta V} \int_{\Delta V'} \int_{k} \int_{k'} e^{i(kr-k'r')} \langle \hat{S}(k) \hat{S}^*(k') \rangle
\]

\[
\uparrow \quad \text{but recall} \quad S(k) \delta(k-k')
\]
\[
\left\langle S_{\Delta V} \hat{S}_{\Delta V'} \right\rangle = \frac{1}{\Delta V^2} \int_{\Delta V} \int_{\Delta V'} \int_{dk} e^{ik \cdot (r-r')} \delta (r-r') S(\hbar) \quad S = \text{const.}
\]

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

\[
\left\langle S_{\Delta V} \hat{S}_{\Delta V'} \right\rangle = \frac{S}{\Delta V^2} \int_{\Delta V} \int_{\Delta V'} \delta (r-r')
\]
\[
\langle S_{\Delta V} S_{\Delta V'} \rangle = \begin{cases} 
\frac{S}{\Delta V} & \text{if } \Delta V = \Delta V' \\
0 & \text{otherwise}
\end{cases}
\]

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

\[
\langle \delta S_{\Delta V}^2 \rangle = \frac{S}{\Delta V} = \frac{m \bar{S}_0}{\Delta V} = m \cdot \frac{(m \bar{N}_p)}{\Delta V}
\]

\[
\langle \delta S_{\Delta V}^2 \rangle = \frac{m^2}{\Delta V^2} \cdot \bar{N}_p \quad \text{since} \quad \langle \delta N_p^2 \rangle = \bar{N}_p \quad \text{Poisson!}
\]
So far we were sloppy with normalization factors for the Fourier transforms. There are different definitions with factors of $(2\pi i)$ placed either in $\exp(2\pi i \xi \Gamma)$, 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 $(2\pi i)$ is considered in $\langle \hat{W}(k_1)\hat{W}^*(k_2) \rangle$ it is OK.
Best is to consider a finite periodic system and use a Fourier series instead of an integral:

\[
\begin{align*}
\hat{S}(k) &= \frac{1}{L^d} \int e^{-i k \cdot r} S(r) \, dr \\
S(r) &= \sum_{k} e^{i k \cdot r} \hat{S}(k) \\
k &= \frac{2 \pi k}{L}, \quad k \in \mathbb{Z}^d
\end{align*}
\]

Analogous definitions exist in the discrete setting, \( \frac{1}{L^d} \leftrightarrow \frac{1}{N_c} \).
Consider white noise \( W(r) \):

\[
\left\langle \hat{W}(k) \hat{W}^*(k') \right\rangle = \frac{1}{L^2} \int \int e^{ik' \cdot (r-r')} \, dr \, dr',
\]

1D for \( r \rightarrow r' \)

\[
= \frac{1}{L^2} \int_0^L \, dr \, e^{ik' \cdot r} = \frac{1}{L^2} \cdot L \cdot \delta_{kk'}
\]

\[
\left\langle \hat{W}(k) \hat{W}^*(k') \right\rangle = \frac{1}{V} \delta_{kk'}
\]

system volume \( V \)
This calculation shows that in any orthonormal basis the weights (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 cylindrical Brownian motion or Brownian sheets and the SPDEs (at least linearized). In the non-linear 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 truncating Fourier space representations to the first \( N_c \) modes (wavenumbers).

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

\[
\langle W_{\Delta V} W_{\Delta V}' \rangle = \langle W_{\Delta V}^2 \rangle \delta_{\Delta V, \Delta V'}
\]

\[
\langle W_{\Delta V}^2 \rangle = N_c \langle \hat{W} \hat{W}^* \rangle = \frac{1}{\Delta V} \quad \text{as before}
\]
We can thus judge how good a discretization is by examining the discrete structure factor at equilibrium.

\[ S(k) = \sqrt{\left< \hat{S}(k) \hat{S}^*(k) \right> = 1 \text{ (ideally)} \]

which implies the correct covariance in real space:

\[ \left< (\delta S_i)(\delta S_j) \right> = \frac{m \delta_{0}}{\Delta V} \delta_{i,j} \]
When discretizing white noise, what we are doing is truncating the spectrum at wavenumber \( k_{\text{max}} = \frac{\pi}{\Delta x} \), or equivalently, representing \( W(r,t) \) with its space-time finite-volume average

\[
\frac{1}{\Delta x \Delta t} \int \int W(r,t) \, dr \, dt \iff \frac{n}{\sqrt{\Delta x \cdot \Delta t}} \mathcal{N} \sim W_i
\]

where \( \mathcal{N} \) is a normally-distributed (Gaussian) unit random variate.
The continuum SPDE

\[
\begin{aligned}
\partial_t u &= \chi \nabla^2 u + \sqrt{2} \chi x \cdot (\nabla \cdot W) \\
&= L u + K W
\end{aligned}
\]

where \( L = \chi \nabla^2 \) and \( K = \sqrt{2} \chi x \cdot \nabla \) are linear differential operators.

Or, in Fourier space

\[
\begin{aligned}
\partial_t \hat{u} &= -\chi k^2 \hat{u} + \sqrt{2} \chi x \cdot (ik) \hat{W} \\
&= \hat{L} \hat{u} + \hat{K} \hat{W}
\end{aligned}
\]
A spatial discretization of this stochastic diffusion equation would have the form

$$\partial_t \mathbf{u} = L \mathbf{u} + K \widetilde{\nabla}$$

where $L$ is now a discrete Laplacian,

E.g.,

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

and $K$ is a discrete divergence, e.g.,

$$\left( K \widetilde{\nabla} \right)_i = \frac{\widetilde{n}_{i+1} - \widetilde{n}_{i-1}}{2 \Delta x}$$

$\triangleq$ Sandra's talk
For periodic boundary conditions, we can use a discrete Fourier transform to translate to

\[ \hat{2_t \hat{u}} = \hat{L} \hat{u} + \hat{K} \hat{\omega} \]

"symbols" of \( L \) and \( K \)

\[
\begin{align*}
\hat{L} &= e^{-2 + e} \\
\hat{K} &= e^{-e} \frac{i k \Delta x}{\Delta x^2} - e^{-i k \Delta x} \frac{1}{2 \Delta x}
\end{align*}
\]
In all cases, discrete or continuous, or real space or Fourier space, we have a simple SDE with additive noise:

$$\partial_t u = Lu + KW$$

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

The basic property at equilibrium is the steady-state covariance.
\[ C = \langle uu^* \rangle \quad \text{equilibrium ensemble} \]
(or time average by ergodicity argument)

First approach is to look at the function:

\[ C (u(r,t)) = C(u) = uu^* \]

and use Itô's formula or the Backward Kolmogorov equation

\[ \partial_t C = (Lu) \cdot \partial_u C + \frac{1}{2} (KK^*) \cdot \partial_{uu} C = 0 \]

BVP

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

\[
\left[ (L \nu) \cdot \frac{\partial}{\partial u} (\mu \nu^*) \right]_{jk} = (L \nu)_i \ \frac{\partial}{\partial u_i} (\mu_j \nu_k)
\]

\[
= \text{Lie}_\nu \left[ \delta_{ij} \nu_k + \delta_{ik} \nu_j \right] =
\]

\[
= \text{Lie}_\nu \nu_k + \nu_j \nu_k L^*_{k j}
\]

\[
= \text{Lie}_\nu \nu_k + \nu_j \nu_k L^*_{k j} = \text{Lie}_\nu \nu_k + \nu_j \nu_k L^*
\]

(Note that \( C^* = C \))
Similarly, \( \frac{1}{2} (KK^*) \cdot \frac{\partial}{\partial u} (uu^*) = KK^* \)

So we get the linear system or linear boundary-value problem:

\[
L C + C L^* = KK^*
\]

At thermodynamic equilibrium, recall that for the simple diffusion equation \( u \equiv 0 \) we have

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

\( \equiv \) identity
This gives the fluctuation-dissipation balance condition:

\[ L + L^* = \frac{\Delta V}{S} KK^* \]

Recall:

\[
\begin{align*}
\partial_t u &= \nabla^2 u + \sqrt{2xS} \mathcal{D} \left( \frac{v}{\sqrt{\Delta V}} \right) \\
\text{discrete Laplacian} &
\end{align*}
\]

\[ L = \nabla^2, \quad K = \sqrt{\frac{2xS}{\Delta V}} \mathcal{D} \]

Note DFDDB is satisfied if:

\[ L = DD^* \]
It is not too hard to construct spatial discretizations that obey this condition, as we will discuss next time.

We can also easily include advection in this picture, i.e., consider the advection-diffusion equation:

\[ \partial_t g + \mathbf{v} \cdot \nabla g = \nabla^2 g + \sqrt{2} s \cdot \nabla W(r,t) \]

where \( \mathbf{v} \) is a specified (constant) velocity field \( \nabla \cdot \mathbf{v} = 0 \).
New \[ L = \nabla^2 + \mathbf{u} \cdot \nabla \]
\[ = \nabla^2 + A(\mathbf{u}) \]
\[ \text{advection operator} \]

Note that \[ L + L^* = 2\nabla \mathcal{L} = \frac{\Delta V}{S} \]

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

\[ A^*(\mathbf{u}) = -A(\mathbf{u}) \]

\[ \text{advection does not dissipate or amplify fluctuations} \]
This follows from
\[ \int_{\Omega} w \left[ \mathbf{v} \cdot \nabla \mathbf{c} \right] \, d\mathbf{r} = \int_{\Omega} w \cdot \left[ \mathbf{v} \mathbf{w} \right] \, d\mathbf{r} \]
\[ = - \int_{\Gamma} \mathbf{c} \cdot \left[ \mathbf{w} \mathbf{v} \right] \, d\mathbf{r} = - \int_{\Gamma} \mathbf{c} \cdot \left[ \mathbf{v} \cdot \mathbf{n} \mathbf{w} \right] \, d\mathbf{r} \]

under periodic boundary conditions or no-slip BCs:
\[ \nabla \cdot \mathbf{v} = 0 \quad \text{in} \ 2\Omega, \quad \mathbf{v} \cdot \mathbf{n} = 0 \]

Similarly, \( \nabla^* = - \nabla \) since
\[ \int_{\Omega} w \left( \nabla \cdot \mathbf{v} \right) \, d\mathbf{r} = - \int_{\Omega} \mathbf{v} \cdot \nabla w \, d\mathbf{r} \]
A spatio-temporal discretization could be based on the Euler scheme (really Euler-Maryama).

\[ u^{n+1} = u^n + xL^2 u^n \Delta t + \sqrt{\frac{2xS \Delta t}{\Delta V}} DW \]

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.