On diffusion and wave front propagation in narrow random channels.

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Motivation : molecular motors.

- We can think of Brownian motors/ratchets as particles (which model the protein molecules) traveling along a designated track.
- At a microscopic scale such a motion is conveniently described as a diffusion process with a deterministic drift.
- On the other hand, the designated track along which the molecule is traveling can be viewed as a tubular domain of some random shape.
- In particular, such a domain can have many random wings added to it.
**Fig. 1**: A model of the molecular motor.
Mathematical modeling: The domain $D$.

- $h_0^\pm(x)$-height functions. They are a pair of piecewise smooth functions with $h_0^+(x) - h_0^-(x) = l_0(x) > 0$.

- The "main channel"

$$D_0 = \{(x, z) : x \in \mathbb{R}, h_0^-(x) \leq z \leq h_0^+(x)\}$$

is a tubular 2-d domain of infinite length, i.e. it goes along the whole $x$-axis. At the discontinuities of $h_0^\pm(x)$, we connect the pieces of the boundary via straight vertical lines.

- Let a sequence of "wings" $D_j$ ($j \geq 1$) be attached to $D_0$. These wings are attached to $D_0$ at the discontinuities of the functions $h_0^\pm(x)$.

- The union $D = D_0 \cup \left( \bigcup_{j=1}^{\infty} D_j \right)$ models the designated track along which the motor is traveling.
**Fig. 1:** A model of the molecular motor.
Mathematical modeling: The domain $D$.

- We can make some standard regularity assumptions about the shape of $D$.
- The shape of the domain $D$ is random.
- **Stationarity**: $P(A) = P(\theta_r(A))$.
- **Mixing**: For any $A \in \mathcal{F}_s^t$ and any $B \in \mathcal{F}_{s+r}^{t+r}$ we have
  \[
  \lim_{r \to \pm \infty} |P(A \cap B) - P(A)P(B)| = 0
  \]
  exponentially fast.

  For instance, we can assume that there exists some $M > 0$ such that $P(A \cap B) = P(A)P(B)$ for $|r| \geq M$. 
In many problems it is natural to assume that the domain $D$ is a thin and long channel.

We "shrink" $D$. Let $D^\varepsilon = \{(x, \varepsilon z) : (x, z) \in D\}$. The parameter $\varepsilon > 0$ is small.
**Fig. 1:** A model of the molecular motor.
The motor (protein molecule) is a diffusion particle moving inside $D^\varepsilon$.

Consider the diffusion process $\hat{X}^\varepsilon_t = (\hat{X}^\varepsilon_t, \hat{Z}^\varepsilon_t)$ in the domain $D^\varepsilon$, which is described by the following system of stochastic differential equations:

\begin{align*}
  d\hat{X}^\varepsilon_t &= dW_1^t + V(\hat{X}^\varepsilon_t, \hat{Z}^\varepsilon_t/\varepsilon)dt + \nu_1(\hat{X}^\varepsilon_t, \hat{Z}^\varepsilon_t)d\hat{\ell}^\varepsilon_t, \\
  d\hat{Z}^\varepsilon_t &= dW_2^t + \nu_2(\hat{X}^\varepsilon_t, \hat{Z}^\varepsilon_t)d\hat{\ell}^\varepsilon_t.
\end{align*}

(1)
Mathematical modeling: The diffusion particle.

- Scalar field $V(x, z) > 0, (x, z) \in D$ characterizes the speed of the transportation in the $x$-direction.

- Vector field $\nu = (\nu_1, \nu_2)$ on $\partial D^\varepsilon$ is defined as the inward unit normal vector at the corresponding point on $\partial D$: $\nu(x, \varepsilon z) = n(x, z)$ when $(x, z) \in \partial D$.

- The process $(W_t^1, W_t^2)$ is a standard 2-dimensional Wiener process independent of the shape of $D$. In other words our process $\hat{X}_t^\varepsilon$ is moving in an independent random environment characterized by random shape of the domain $D$.

- The process $\hat{\ell}_t^\varepsilon$ is the local time of the process $\hat{X}_t^\varepsilon$ at $\partial D^\varepsilon$. 
Equivalent formulation in $D$. 

- Recall that the diffusion process $\hat{X}_t^\varepsilon = (\hat{X}_t^\varepsilon, \hat{Z}_t^\varepsilon)$ is moving in the domain $D^\varepsilon$.
- We can make a change of variable $\hat{Z}_t^\varepsilon \to \hat{Z}_t^\varepsilon / \varepsilon = Z_t^\varepsilon$ in the equation (1):

\[
\begin{cases}
    d\hat{X}_t^\varepsilon = dW_1^t + V(\hat{X}_t^\varepsilon, \hat{Z}_t^\varepsilon / \varepsilon)dt + \nu_1(\hat{X}_t^\varepsilon, \hat{Z}_t^\varepsilon)d\ell_t^\varepsilon, \\
    d\hat{Z}_t^\varepsilon = dW_2^t + \nu_2(\hat{X}_t^\varepsilon, \hat{Z}_t^\varepsilon)d\ell_t^\varepsilon.
\end{cases}
\]

(1)

- We then equivalently consider the diffusion process $X_t^\varepsilon = (X_t^\varepsilon, Z_t^\varepsilon)$ in the original domain $D$ as follows:

\[
\begin{cases}
    dX_t^\varepsilon = dW_1^t + V(X_t^\varepsilon, Z_t^\varepsilon)dt + \nu_1^\varepsilon(X_t^\varepsilon, Z_t^\varepsilon)d\ell_t^\varepsilon, \\
    dZ_t^\varepsilon = \frac{1}{\varepsilon}dW_2^t + \nu_2^\varepsilon(X_t^\varepsilon, Z_t^\varepsilon)d\ell_t^\varepsilon.
\end{cases}
\]

(2)
Notational convention.

- \( P, E \) with respect to the random shape of \( D \). (the environment)
- \( P^W, E^W \) with respect to the driving noise \((W_t^1, W_t^2)\).
The process $X_t^\varepsilon$: fast and slow components.

▶ We recall (2):

\[
\begin{align*}
    dX_t^\varepsilon &= dW_t^1 + V(X_t^\varepsilon, Z_t^\varepsilon)dt + \nu_1^\varepsilon(X_t^\varepsilon, Z_t^\varepsilon) d\ell_t^\varepsilon, \\
    dZ_t^\varepsilon &= \frac{1}{\varepsilon} dW_t^2 + \nu_2^\varepsilon(X_t^\varepsilon, Z_t^\varepsilon) d\ell_t^\varepsilon, 
\end{align*}
\]

(2)

▶ The process $X_t^\varepsilon$ has the "fast" and the "slow" components. The "fast" component is the process $Z_t^\varepsilon$ and the "slow" component is the process $X_t^\varepsilon$. 
According to the averaging principle we can expect a mixing in the "fast" component before the "slow" component $X_t^\varepsilon$ changes significantly. We shall describe the limiting slow motion.

Problems of this type initiated in Freidlin–Wentzell, PTRF, 2012. ("fish paper")
Fig. 1: A model of the molecular motor.
Averaging principle : Result.

- We fix a random shape of $D$. ("quenched" setting) After that we allow the shape of $D$ be random and we will work on a corresponding random graph.

- Introduce the metric graph $\Gamma$ corresponding to the domain $D$. Introduce the projection map $\mathcal{Y}$.

- We can show similarly as in the previously mentioned paper of Freidlin–Wentzell that as $\varepsilon \downarrow 0$, the process $\mathcal{Y}(X_t^\varepsilon)$ converges weakly in $C_{[0,T]}(\Gamma)$ to a Markov process $Y_t$ on $\Gamma$.

- In other words we have

$$
E^W_{X_0^\varepsilon = x} F(\mathcal{Y}(X_t^\varepsilon)) \rightarrow E^W_{\mathcal{Y}(x)} F(Y_t)
$$

for every bounded continuous functional $F$ on the space $C_{[0,T]}(\Gamma)$.
Averaging principle: The process $Y_t$.

- The process $Y_t$ is a diffusion process on $\Gamma$ with a generator $A$ and the domain of definition $D(A)$.
- For each edge $I_k$ we define an operator $\bar{L}_k$:

$$\bar{L}_k u(x) = \frac{1}{2l_k(x)} \frac{d}{dx} \left( l_k(x) \frac{du}{dx} \right) + \bar{V}_k(x) \frac{du}{dx}, \quad A_k \leq x \leq B_k.$$
Averaging principle: The process $Y_t$.

Here

$$\overline{V}_k(x) = \frac{1}{l_k(x)} \int_{h_k^{-}(x)}^{h_k^{+}(x)} V(x, z) dz$$

is the average of the velocity field $V(x, z)$ on the connected component $C_k(x)$, with respect to Lebesgue measure in $z$-direction. At places where $l_k = 0$, the above expression for $\overline{V}_k(x)$ is understood as a limit as $l_k \to 0$:

$$\overline{V}_k(x) = \lim_{y \to x} \frac{1}{l_k(y)} \int_{h_k^{-}(y)}^{h_k^{+}(y)} V(y, z) dz .$$

We assume for simplicity $\overline{V}_k(x) = \beta > 0$ is a constant.
Averaging principle: The process $Y_t$.

- The operator $A$ is acting on functions $f$ on the graph $\Gamma$: for $y = (x, k)$ being an interior point of the edge $l_k$ we take $Af(y) = \overline{L}_k f(x, k)$.
- What about the domain $D(A)$ (boundary conditions)?
- We introduce

$$q_k(x) = \int \frac{dx}{l_k(x)} \quad , \quad r_k(x) = 2 \int l_k(x) dx .$$

(scale function and speed measure)
The domain of definition $D(A)$ of the operator $A$ consists of such functions $f$ satisfying the following properties.

- The function $f$ must be a continuous function that is twice continuously differentiable in $x$ in the interior part of every edge $I_k$;
- There exist finite limits $\lim_{y \to O_i} Af(y)$ (which are taken as the value of the function $Af$ at the point $O_i$);
Averaging principle: The process $Y_t$.

- One more property.
  - There exist finite one-sided limits $\lim_{x \to x_i} D_{q_k} f(x, k)$ along every edge ending at $O_i = (x_i, k)$ and they satisfy the gluing conditions

$$
\sum_{j=1}^{N_i} (\pm) \lim_{x \to x_i} D_{q_{k_j}} f(x, k_j) = 0, \quad (3)
$$

where the sign "+" is taken if the values of $x$ for points $(x, k_j) \in I_{k_j}$ are $\geq x_i$ and "−" otherwise. Here $N_i = 1$ (when $O_i$ is an exterior vertex) or 3 (when $O_i$ is an interior vertex).
Averaging principle: The process $Y_t$.

- For an exterior vertex $O_i = (x_i, k)$ with only one edge $l_k$ attached to it the condition (3) is just $\lim_{x \to x_i} D_{q_k} f(x, k) = 0$.

- For an interior vertex the gluing condition (3) can be written with the derivatives $\frac{d}{dx}$ instead of $D_{q_k}$. For $k$ being one of the $k_j$ we define $\alpha_{i,k} = \lim_{x \to x_i} l_k(x)$ (for each edge $l_k$ the limit is a one-sided one). Then the condition (3) can be written as

$$
\sum_{j=1}^{3} (\pm) \alpha_{i,k_j} \cdot \lim_{x \to x_i} \frac{df(x, k_j)}{dx} = 0 .
$$

(4)
Fig. 1: A model of the molecular motor.
An interesting question arising in the applications is to calculate the effective speed of the particles.

In mathematical language this problem can be formulated as follows. Let $\sigma^\varepsilon((\infty, a])$ be the first time that the process $X^\varepsilon_t$, starting from a point $x_0 = (x_0, z_0) \in D$, hits $D \cap \{x = a > 0\}$. The limit

$$\lim_{a \to \infty} \lim_{\varepsilon \downarrow 0} \frac{\sigma^\varepsilon((\infty, a])}{a}$$

exists in $P \times P^W_{(x_0, z_0)}$-probability and can be viewed as the inverse of the average effective speed of transportation of the particle inside $D$. 
Answer.

Theorem. (Freidlin–H, JSP, 2013, to appear) We have

\[
\lim_{a \to \infty} \lim_{\varepsilon \downarrow 0} \frac{\sigma^\varepsilon((-\infty, a])}{a} = 2 \int_0^\infty K(t) \exp(-2\beta t) dt + 2 \mathbb{E} n \mathbb{E} \text{sign}(r) \int_0^r l_{\text{wing}}(t) \exp(2\beta t) dt \int_0^\infty \frac{1}{l_0(y)} \exp(-2\beta y) dy
\]

in probability. Here \( K(t) = \mathbb{E} \frac{l_0(s)}{l_0(s + t)} \).
Brief sketch of the calculation.

- We first consider the corresponding Markov time $\tau((-\infty, a])$ for the limiting process $Y_t$.
- **Step 1.** "average transportation time when there is no wing"

$$
\lim_{a \to \infty} \frac{E_0^W \tau((-\infty, a])}{a} = 2 \int_0^\infty K(t) \exp(-2\beta t) dt,
$$

where $K(t) = E \frac{l_0(s)}{l_0(s + t)}$. 

Fig. 2: The case when $l_0(x)$ has jumps.
Brief sketch of the calculation.

- **Step 2.** "average transportation time inside $D_0"$ Do an approximation.

\[
\lim_{a \to \infty} \frac{\mathbb{E}_W^W \int_0^{\tau((-\infty, a])} \mathbf{1}(\mathcal{Y}^{-1}(Y_t) \subset D_0) \, dt}{a} = 2 \int_0^\infty K(t) \exp(-2\beta t) \, dt
\]

where $K(t) = \mathbb{E} \frac{l_0(s)}{l_0(s + t)}$. 
Brief sketch of the calculation.

▶ Step 3. ”average transportation time spent in one wing” First we let this wing be located at $x = 0$.

$$E_0^W \tau_{I_3}((−\infty, a])$$

$$= 2\text{sign}(r) \int_0^r l_3(t) \exp(2\beta t)dt \int_0^a \frac{1}{l_2(y)} \exp(-2\beta y)dy .$$
Brief sketch of the calculation.

- **Step 3 (continued).** "average transportation time spent in one wing" Let this wing be located at \( x = q \). If \( q > 0 \) then

\[
E^W_0 \tau_{l_3}((−∞, a])
= 2 \text{sign}(r) \int_{q}^{q+r} l_3(t) \exp(2\beta(t - q))dt \times \\
\int_{q}^{a} \frac{1}{l_2(y)} \exp(-2\beta(y - q))dy .
\]

If \( q < 0 \) then

\[
E^W_0 \tau_{l_3}((−∞, a])
= 2 \text{sign}(r) \int_{q}^{q+r} l_3(t) \exp(2\beta(t - q))dt \times \\
\int_{0}^{a} \frac{1}{l_2(y)} \exp(-2\beta(y - q))dy .
\]
Brief sketch of the calculation.

▶ **Step 4.** ”average transportation time spent in all wings” We have

\[
\lim_{a \to \infty} \mathbb{E}_0^W \int_0^{\tau(-\infty,a]} 1(\mathcal{Y}^{-1}(Y_t) \notin D_0) dt
\]

\[
= 2\mathbb{E} n \mathbb{E}_{\text{sign}(r)} \int_0^r a l_{\text{wing}}(t) \exp(2\beta t) dt \int_0^{\infty} \frac{1}{l_0(y)} \exp(-2\beta y) dy
\]

in probability.
Brief sketch of the calculation.

▶ **Step 5.** Combine Steps 2 and 4 we have

\[
\lim_{a \to \infty} \lim_{\varepsilon \downarrow 0} \frac{E_{x_0}^W \sigma^\varepsilon((-\infty, a])}{a} = 2 \int_0^{\infty} K(t) \exp(-2\beta t) dt
\]

\[
+ 2 E_{nE} \text{sign}(r) \int_0^r l_{\text{wing}}(t) \exp(2\beta t) dt \int_0^{\infty} \frac{1}{l_0(y)} \exp(-2\beta y) dy
\]

in probability. Here \( K(t) = E \frac{l_0(s)}{l_0(s + t)}. \)
Brief sketch of the calculation.

- **Step 6.** Conclude that

\[ \lim_{a \to \infty} \lim_{\varepsilon \downarrow 0} \frac{E_{x_0}^W \sigma^\varepsilon ((-\infty, a])}{a} = \lim_{a \to \infty} \lim_{\varepsilon \downarrow 0} \frac{\sigma^\varepsilon ((-\infty, a])}{a}. \]

(”*Bernstein argument*” and \( \beta > 0 \))
Remarks and Generalizations.

- Multidimensional situation.
- The case when random shape of $D$ depends on time: "ratchet effect".
- More general graphs.
Fig. 3: A more general graph.
Reaction-diffusion equation in narrow random channels.

\[ \begin{align*}
\frac{\partial u^\varepsilon}{\partial t} &= \frac{1}{2} \left( \frac{\partial^2 u^\varepsilon}{\partial x^2} + \frac{\partial^2 u^\varepsilon}{\partial z^2} \right) + V(x, z) \frac{\partial u^\varepsilon}{\partial x} + f(u^\varepsilon), \\
\partial_{\nu} u^\varepsilon \bigg|_{\partial \Omega^\varepsilon} &= 0, \\
u^\varepsilon &= u^\varepsilon(t, x, z), (t, x, z) \in \mathbb{R}_+ \times \Omega^\varepsilon.
\end{align*} \]
Reactor-diffusion equation in narrow random channels.

- Same as before, we rescale $D^\varepsilon \rightarrow D$:

\[
\frac{\partial u^\varepsilon}{\partial t} = \frac{1}{2} \left( \frac{\partial^2 u^\varepsilon}{\partial x^2} + \frac{1}{\varepsilon^2} \frac{\partial^2 u^\varepsilon}{\partial z^2} \right) + V(x, z) \frac{\partial u^\varepsilon}{\partial x} + f(u^\varepsilon),
\]

\[
\begin{align*}
&u^\varepsilon(0, x, z) = g(x), \\
&\frac{\partial u^\varepsilon}{\partial n^\varepsilon} \bigg|_{\partial D} = 0, \\
&u^\varepsilon = u^\varepsilon(t, x, z), \ (t, x, z) \in \mathbb{R}_+ \times D.
\end{align*}
\]

- $f(u)$ is of KPP type nonlinearity; $g(x) \geq 0$ (not identically equal to 0) smooth and compactly supported.
Reaction-diffusion equation in narrow random channels.

- Path integral representation (Feynmann-Kac) formula for the generalized solution:

\[
\begin{align*}
    u^\varepsilon(t, (x, z)) &= \mathbb{E}_{(x, z)}^W \left[ \exp \left( \int_0^t c(u^\varepsilon(t - s, X_s^\varepsilon)) ds \right) g(X_t^\varepsilon) \right].
\end{align*}
\]

- Here \( c(u) = \frac{f(u)}{u} \) for \( u > 0 \) and \( c(0) = \lim_{u \downarrow 0} \frac{f(u)}{u} = \sup_{u > 0} \frac{f(u)}{u} \).

The latter equality is due to the KPP nonlinearity assumption.

We shall also suppose that \( |c'(u)| \leq \text{Lip}(c) < \infty, \ u \in [0, 1] \).

- The proof of existence, uniqueness and regularity of the generalized solution to the integral equation (7) is close to Freidlin, 1985, red book, Chapter 5, Section 3.
Approximation by a RDE on random graph.

- Making use of the convergence of $\mathcal{Y}(X^\varepsilon_t)$ to $Y_t$ as $\varepsilon \downarrow 0$ we have

$$\lim_{\varepsilon \downarrow 0} \max_{0 \leq t \leq T} \max_{(x,z) \in D} |u^\varepsilon(t, (x, z)) - u(t, \mathcal{Y}((x, z))))| = 0.$$ 

- Here $u(t, y), t \geq 0, y = (x, k) \in \Gamma$ is the generalized solution to the RDE on $\Gamma$:

$$\frac{\partial u}{\partial t} = Au + f(u), u(0, (x, k)) = g(x), u(t, \bullet) \in D(A), (t, y) \in \mathbb{R}_+ \times \Gamma.$$ 

- Feynmann-Kac formula :

$$u(t, (x, k)) = E^{W}_{(x,k)} \left[ \exp \left( \int_{0}^{t} c(u(t - s, Y_s))ds \right) g(X_t) \right].$$ (8)
We then focus on \( u(t, (x, k)) \).

The study of wave front propagation for RDE in random environment was first initiated by Freidlin–Gärtner, 1979. They considered there a 1-d situation with no drift.

The case of 1-d with the presence of a drift was considered by Nolen–Xin (CMP 2007, Dis Cont Dyn Sys B. 2009). They assume that the mean drift is 0.

We mainly follow the technique developed in Nolen–Xin. As a consequence we shall assume that the mean drift \( \beta = 0 \).
Wave front propagation.

\[ \mu^\pm(\lambda) \equiv \frac{1}{EL} E \left( \ln E^W [e^{\lambda T_0^\pm L} \mathbb{1}_{T_0^\pm L < \infty}] \right). \]

\[ I^\pm(a) \equiv \sup_{\lambda \leq 0} (a\lambda - \mu^\pm(\lambda)). \]

We define non-random constants \( c^*_+ > 0 \) and \( c^*_- < 0 \) as the solutions of the equations

\[ c^*_+ I^+ \left( \frac{1}{c^*_+} \right) = f'(0), \]

\[ |c^*_-| I^- \left( \frac{1}{|c^*_-|} \right) = f'(0). \]

These solutions exist and are unique.
Wave front propagation.

> Theorem. (Freidlin-H, preprint, 2013) For any closed set $F \subset (-\infty, c^-) \cup (c^+, \infty)$ we have

$$\lim_{t \to \infty} \sup_{c \in F} u(t, (ct, k)) = 0$$

almost surely with respect to $P$. For any compact set $K \subset (c^-, c^+)$ we have

$$\lim_{t \to \infty} \inf_{c \in K} u(t, (ct, k)) = 1$$

almost surely with respect to $P$. 
Basic ingredients in the proof.

- The main technique of the proof borrows from Nolen–Xin (2007, 2009).
- Actually all these results are based on the large deviation approach suggested in Freidlin–Gärtner, 1979.
- We have more degrees of freedom due to the presence of the wings.
- LDP is a large scale effect so that finite length of wings do not affect the analysis.
Basic ingredients in the proof.

- We need to show finiteness of the Lyapunov exponents
  \[ E[|\ln E^W[e^{-\lambda T_0^L}]|] < \infty; \ E[|\ln E^W[e^{-\lambda T_0^{-L}}]|] < \infty. \]

- This is done by considering the solution of the Sturm-Liouville problem
  \[ Au - \lambda u = 0 \text{ on } \Gamma, \ u \in D(A), \ u(0) = 1, \ u(+\infty) = 0. \]

- We make use of Feller’s theory and the structure of the random graph \( \Gamma \).
**Fig. 1:** A model of the molecular motor.
Basic ingredients in the proof.

- Products of random matrices naturally appear in the analysis.
- However these matrices contain negative terms so that it is not easy to analyze the limit of the products.
- We can show finiteness of Lyapunov exponents so that we can conclude existence of wave speed.
Questions left open.

- Identify/estimate the wave speed. This needs more information about the limit of products of random matrices appeared in our problem. To this end probably Markov dependence assumption is needed and the limit point is identified as certain boundary point.

- The case $\beta > 0$ as in the molecular motors. We do not know how to deal with this case yet...
The end.

- Thank you for your attention!