Effective dynamics for stochastic differential equations

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Motivation: entropic force for polymer chains

Let us recall the basic micro-macro model for polymeric fluids.

We consider a dilute solution of polymers, with polymer chains which are:

1. very numerous (statistical mechanics),
2. small and light (Brownian effects),
3. within a Newtonian solvent.

Macroscopic level

Momentum equations (incompressible fluid):

$$\rho\left(\partial_t + \mathbf{u}.\nabla\right)\mathbf{u} = -\nabla p + \mathrm{div}\,(\boldsymbol{\sigma}) + \mathbf{f}_{ext},$$

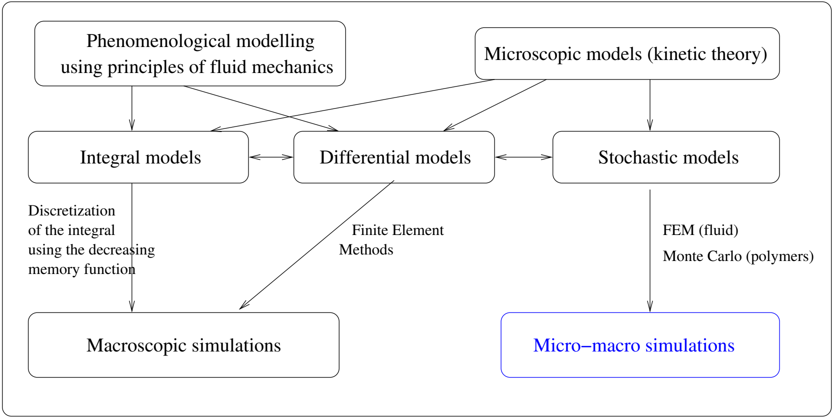
$$\mathrm{div}\,(\mathbf{u}) = 0.$$

Non-Newtonian fluids:

$$\boldsymbol{\sigma} = \eta\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right) + \boldsymbol{\tau},$$

where the extra-stress $\boldsymbol{\tau}$ depends on *the history of the deformation*.

Multiscale modeling



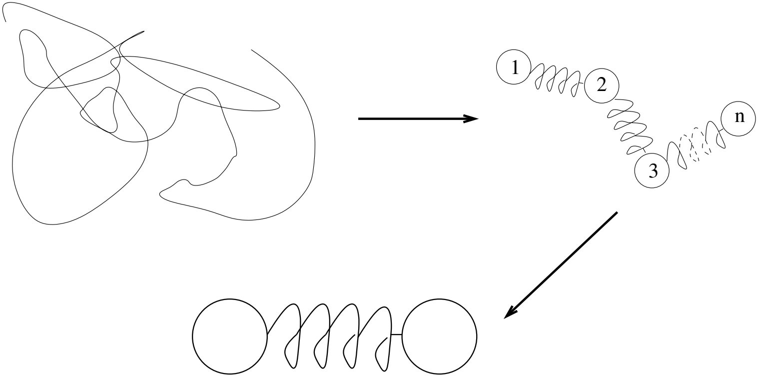
Differential models : $\frac{D\boldsymbol{\tau}}{Dt} = f(\boldsymbol{\tau}, \nabla \mathbf{u}),$

Integral models : $\boldsymbol{\tau} = \int_{-\infty}^{t} m(t-t')\mathbf{S}_t(t')\,dt'.$

(Macroscopic approach: R. Keunings & al., B. van den Brule & al., M. Picasso & al.)

Microscopic model (1/4)

A coarse-grained description: consider blobs (1 blob $\simeq$ 20 CH_2 groups). The basic model (the dumbbell model): only two blobs. The conformation is given by the "end-to-end vector".



References: R.B. Bird, C.F. Curtiss, R.C. Armstrong and O. Hassager, *Dynamic of Polymeric Liquids*, Wiley / M. Doi, S.F. Edwards, *The theory of polymer dynamics*, Oxford Science Publication) / H.C. Öttinger, *Stochastic processes in polymeric fluids*, Springer.

Microscopic model (2/4)

Forces on bead i ($i = 1$ or 2) of coordinate vector $\boldsymbol{X}_t^i$ in a velocity field $\mathbf{u}(t, \boldsymbol{x})$ of the solvent (zero mass Langevin equation):

- Drag force: $$-\zeta \left(\frac{d\boldsymbol{X}_t^i}{dt} - \mathbf{u}(t, \boldsymbol{X}_t^i) \right),$$
- Entropic force on bead i: $\mathbf{F}^1 = -\mathbf{F}^2 = \mathbf{F}(\boldsymbol{X}_t^2 - \boldsymbol{X}_t^1)$. For example:
$$\mathbf{F}(\boldsymbol{X}) = H\boldsymbol{X} \text{ (Hookean dumbbell)},$$
$$\mathbf{F}(\boldsymbol{X}) = \frac{H\boldsymbol{X}}{1 - \|\boldsymbol{X}\|^2/(bkT/H)} \text{ (FENE dumbbell)}.$$
- "Brownian force": $$\sqrt{2kT\zeta}\, d\mathbf{B}_t^i$$
with $\mathbf{B}_t^i$ a Brownian motion.

Microscopic model (3/4)

We have:

$$\begin{cases} d\boldsymbol{X}_t^1 = \mathbf{u}(t, \boldsymbol{X}_t^1)\, dt + \zeta^{-1}\mathbf{F}(\boldsymbol{X}_t)\, dt + \sqrt{2kT\zeta^{-1}} d\mathrm{B}_t^1 \\ d\boldsymbol{X}_t^2 = \mathbf{u}(t, \boldsymbol{X}_t^2)\, dt - \zeta^{-1}\mathbf{F}(\boldsymbol{X}_t)\, dt + \sqrt{2kT\zeta^{-1}} d\mathrm{B}_t^2 \end{cases}$$

Let us introduce the end-to-end vector $\boldsymbol{X}_t = \left(\boldsymbol{X}_t^2 - \boldsymbol{X}_t^1\right)$ and the position of the center of mass $\mathrm{R}_t = \frac{1}{2}\left(\boldsymbol{X}_t^1 + \boldsymbol{X}_t^2\right)$:

$$\begin{cases} d\boldsymbol{X}_t = \left(\mathbf{u}(t, \boldsymbol{X}_t^2) - \mathbf{u}(t, \boldsymbol{X}_t^1)\right)\, dt - 2\zeta^{-1}\mathbf{F}(\boldsymbol{X}_t)\, dt + 2\sqrt{kT\zeta^{-1}} d\boldsymbol{W}_t^1, \\ d\boldsymbol{R}_t = \dfrac{1}{2}\left(\mathbf{u}(t, \boldsymbol{X}_t^1) + \mathbf{u}(t, \boldsymbol{X}_t^2)\right)\, dt + \sqrt{kT\zeta^{-1}} d\boldsymbol{W}_t^2, \end{cases}$$

where $\boldsymbol{W}_t^1 = \frac{1}{\sqrt{2}}\left(\boldsymbol{B}_t^2 - \boldsymbol{B}_t^1\right)$ and $\boldsymbol{W}_t^2 = \frac{1}{\sqrt{2}}\left(\boldsymbol{B}_t^1 + \boldsymbol{B}_t^2\right)$.

Microscopic model (4/4)

Approximations:

- $\mathbf{u}(t, \boldsymbol{X}_t^i) \simeq \mathbf{u}(t, \mathrm{R}_t) + \nabla \mathbf{u}(t, \mathrm{R}_t)(\boldsymbol{X}_t^i - \mathrm{R}_t)$,
- the noise on R_t is negligible.

We finally get

$$\begin{cases} d\boldsymbol{X}_t = \nabla \mathbf{u}(t, \boldsymbol{R}_t)\boldsymbol{X}_t\, dt - \dfrac{2}{\zeta}\mathbf{F}(\boldsymbol{X}_t)\, dt + \sqrt{\dfrac{4kT}{\zeta}} d\boldsymbol{W}_t, \\ d\boldsymbol{R}_t = \mathbf{u}(t, \boldsymbol{R}_t)\, dt. \end{cases}$$

Eulerian version: at a fixed macroscopic point $\boldsymbol{x}$

$$d\boldsymbol{X}_t(\boldsymbol{x}) + \mathbf{u}(t, \boldsymbol{x}).\nabla \boldsymbol{X}_t(\boldsymbol{x})\, dt$$
$$= \nabla \mathbf{u}(t, \boldsymbol{x})\boldsymbol{X}_t(\boldsymbol{x})\, dt - \frac{2}{\zeta}\mathbf{F}(\boldsymbol{X}_t(\boldsymbol{x}))\, dt + \sqrt{\frac{4kT}{\zeta}} d\boldsymbol{W}_t.$$

Micro-macro model

The Kramers formula gives the stress tensor $\boldsymbol{\tau}$ in terms of the polymer chain configurations:

$$\boldsymbol{\tau}(t,\boldsymbol{x}) = n_p\Big(-kT\mathrm{Id} + \mathbb{E}\left(\boldsymbol{X}_t(\boldsymbol{x}) \otimes \mathbf{F}(\boldsymbol{X}_t(\boldsymbol{x}))\right)\Big).$$

This yields the complete coupled system:

$$\begin{cases} \rho\left(\partial_t + \mathbf{u}.\nabla\right)\mathbf{u} = -\nabla p + \eta\Delta\mathbf{u} + \mathrm{div}\,(\boldsymbol{\tau}) + \mathbf{f}_{ext}, \\ \mathrm{div}\,(\mathbf{u}) = 0, \\ \boldsymbol{\tau} = n_p\Big(-kT\mathrm{Id} + \mathbb{E}\left(\boldsymbol{X}_t \otimes \mathbf{F}(\boldsymbol{X}_t)\right)\Big), \\ d\boldsymbol{X}_t + \mathbf{u}.\nabla_x\boldsymbol{X}_t\,dt = \left(\nabla\mathbf{u}\boldsymbol{X}_t - \dfrac{2}{\zeta}\mathbf{F}(\boldsymbol{X}_t)\right)\,dt + \sqrt{\dfrac{4kT}{\zeta}}d\boldsymbol{W}_t. \end{cases}$$

Entropic force and coarse-graining

Where does the entropic force come from?
$\mathbf{F}^1 = \nabla_{\boldsymbol{x}^1} \ln \psi_{eq}(\|\boldsymbol{X}_t^2 - \boldsymbol{X}_t^1\|)$, where ψ_{eq} is the equilibrium density of the end-to-end distance $\|\boldsymbol{X}^2 - \boldsymbol{X}^1\|$, in zero velocity field. In statistical physics, this force is called the mean force associated with the collective variable "end-to-end vector".

General question: Starting from dynamics on the full-atom polymer chain $X_t = (X_t^1, \ldots, X_t^n)$ with values in $\mathbb{R}^{3n}$ (n atoms), and the coarse-graining map $\xi(X) = X^n - X^1$ (end-to-end vector), we would like to derive effective Markov dynamics in $\mathbb{R}^3$ close to $(\xi(X_t))_{t \geq 0}$. Is the mean force a good coarse-grained force?

General setting

Let us consider a stochastic dynamics

$$dX_t = -\nabla V(X_t)\, dt + \sqrt{2} dW_t.$$

and a smooth one dimensional function $\xi : \mathbb{R}^d \to \mathbb{R}$. This dynamics admits as an invariant measure:

$$\mu(dx) = Z^{-1} \exp(-V(x))\, dx.$$

Problem: Propose a Markovian dynamics (say on $Z_t \in \mathbb{R}$) that approximates the dynamics $(\xi(X_t))_{t \geq 0}$.

In all what follows, to keep things simple, let us assume that $d = 2$ and

$$\xi(x_1, x_2) = x_1.$$

Free energy

The free energy $A : \mathbb{R} \to \mathbb{R}$ is defined by:

$$\exp(-A(x_1)) = Z^{-1} \int_{\mathbb{R}} \exp(-V(x_1, x_2))\, dx_2.$$

Notice that, $\xi * \mu = \exp(-A(x_1))\, dx_1$: for all test function φ,

$$\int_{\mathbb{R}^2} \varphi \circ \xi \, d\mu = \int_{\mathbb{R}} \varphi(x_1) \exp(-A(x_1))\, dx_1.$$

Question: Is the effective dynamics

$$dZ_t = -A'(Z_t)\, dt + \sqrt{2} dB_t$$

close to $(\xi(X_t))_{t \geq 0} = (X_t^1)_{t \geq 0}$? It is thermodynamically consistent (correct invariant measure) but is it dynamically consistent ?

Construction of the effective dynamics (1/3)

Original dynamics:

- SDE on $X_t = (X_t^1, X_t^2)$:

$$dX_t = -\nabla V(X_t)\, dt + \sqrt{2} dW_t.$$

PDE on $\mathcal{L}(X_t) = \psi(t,x)\, dx = \psi(t, x_1, x_2)\, dx_1 dx_2$:

$$\partial_t \psi = \mathrm{div}\, (\nabla V \psi) + \Delta \psi.$$

Equilibrium: $\psi_\infty = Z^{-1} \exp(-V)$.

- SDE on X_t^1:

$$dX_t^1 = -\partial_1 V(X_t^1, X_t^2)\, dt + \sqrt{2} dW_t^1.$$

PDE on $\mathcal{L}(X_t^1) = \overline{\psi}(t, x_1)\, dx_1$, where $\overline{\psi}(t, x_1) = \int_{\mathbb{R}} \psi(t, x_1, x_2)\, dx_2$:

$$\partial_t \overline{\psi} = \partial_1 \left(\int_{\mathbb{R}} \partial_1 V \psi \, dx_2 \right) + \partial_{1,1} \overline{\psi}.$$

We need a closure approximation.

Construction of the effective dynamics (2/3)

First attempt: Closure by conditional expectation

SDE on $\tilde{z}_t$:

$$d\tilde{Z}_t = -\tilde{b}(t, Z_t)\, dt + \sqrt{2} dW_t^1$$

where

$$\tilde{b}(t,z) = \mathbb{E}(\partial_1 V(X_t^1, X_t^2) | X_t^1 = z) = \frac{\displaystyle\int_{\mathbb{R}} \partial_1 V(x)\psi(t,x) dx_2}{\displaystyle\int_{\mathbb{R}} \psi(t,x) dx_2}.$$

PDE: One has $\mathcal{L}(\tilde{Z}_t) = \overline{\psi}(t, x_1)\, dx_1$! Indeed,

$$\partial_t \overline{\psi} = \partial_1(\tilde{b}\overline{\psi}) + \partial_{1,1}\overline{\psi}$$

since $\displaystyle\int_{\mathbb{R}} \partial_1 V \psi dx_2 = \tilde{b}\,\overline{\psi}$.

But $\tilde{b}$ is not easy to compute... and where is the free energy?

Construction of the effective dynamics (3/3)

Second attempt: Closure by conditional expectation at equilibrium

SDE on Z_t:

$$dZ_t = -b(Z_t)\,dt + \sqrt{2}dW_t^1$$

where

$$b(x_1) = \mathbb{E}_\mu(\partial_1 V(X^1, X^2)|X^1 = x_1) = \frac{\displaystyle\int_{\mathbb{R}} \partial_1 V \exp(-V) dx_2}{\displaystyle\int_{\mathbb{R}} \exp(-V) dx_2}.$$

Notice that, since $A(x_1) = -\ln \int_{\mathbb{R}} \exp(-V)\, dx_2 + \ln Z$,

$$b(x_1) = A'(x_1).$$

PDE on $\mathcal{L}(Z_t) = \phi(t, x_1)\, dx_1$:

$$\partial_t \phi = \partial_1 (A' \phi) + \partial_{1,1} \overline{\phi}.$$

Related approaches: Mori-Zwanzig and projection operator formalism [E/Vanden-Eijnden, ...], asymptotic approaches [Papanicolaou, Freidlin, Pavliotis/Stuart, ...].

Error analysis: time marginals

Theorem [Legoll, TL, 2010]

Let us recall that $\xi(x_1, x_2) = x_1$. Under the assumptions:

(H1) For all x_1, the conditional probability measures $\mu(\cdot|\xi(x) = x_1) = \frac{\psi_\infty(x_1,x_2)dx_2}{\overline{\psi_\infty}(x_1)}$ satisfy a Logarithmic Sobolev Inequality with constant ρ,

(H2) Bounded coupling assumption: $\|\partial_{1,2} V\|_{L^\infty} \leq \kappa$.

Then, if $\mathcal{L}(\xi(X_0)) = \mathcal{L}(Z_0)$, $\exists C > 0$, $\forall t \geq 0$,

$$H(\mathcal{L}(\xi(X_t)), \mathcal{L}(Z_t)) \leq C\frac{\kappa}{\rho}\Big(H(\mathcal{L}(X_0)|\mu) - H(\mathcal{L}(X_t)|\mu)\Big)$$

where $H(\mu|\nu) = \int \ln(d\mu/d\nu)d\mu$ denotes the relative entropy.

Longtime convergence and entropy (1/3)

Recall the original dynamics:

$$dX_t = -\nabla V(X_t)\, dt + \sqrt{2} dW_t.$$

The associated Fokker-Planck equation writes:

$$\partial_t \psi = \mathrm{div}\ (\nabla V \psi) + \Delta \psi.$$

where $X_t \sim \psi(t,x)\, dx$.

The rate of convergence of ψ to $\psi_\infty = Z^{-1} \exp(-V)$ in entropy is dictated by the LSI constant of $\mu(dx) = \psi_\infty(x)\, dx$.

Longtime convergence and entropy (2/3)

Notice that the Fokker-Planck equation rewrites

$$\partial_t \psi = \operatorname{div} \left(\psi_\infty \nabla \left(\frac{\psi}{\psi_\infty} \right) \right)$$

where $\psi_\infty = Z^{-1} \exp(-V)$.

Let us introduce the entropy:

$$H(\psi(t,\cdot)|\psi_\infty) = \int_{\mathbb{R}^2} \ln \left(\frac{\psi}{\psi_\infty} \right) \psi.$$

Longtime convergence and entropy (3/3)

$$\begin{aligned}\frac{dH(\psi(t,\cdot)|\psi_\infty)}{dt} &= \int_{\mathbb{R}^2} \ln\left(\frac{\psi}{\psi_\infty}\right)\partial_t\psi \\ &= \int_{\mathbb{R}^2} \ln\left(\frac{\psi}{\psi_\infty}\right)\mathrm{div}\ \left(\psi_\infty\nabla\left(\frac{\psi}{\psi_\infty}\right)\right) \\ &= -\int_{\mathbb{R}^2}\left|\nabla\ln\left(\frac{\psi}{\psi_\infty}\right)\right|^2\psi =: -I(\psi(t,\cdot)|\psi_\infty).\end{aligned}$$

Definition: The meas $\psi_\infty(x)\,dx$ satisfies a Logarithmic Sobolev Inequality (LSI(R)) iff: $\forall\phi$ pdf,

$$H(\phi|\psi_\infty) \leq \frac{1}{2R} I(\phi|\psi_\infty)$$

Lemma: ψ_∞ satisfies LSI(R) $\iff$ for all IC $\psi(0,\cdot)$, for all $t \geq 0$, $H(\psi(t,\cdot)|\psi_\infty) \leq H(\psi(0,\cdot)|\psi_\infty)\exp(-2Rt)$.

Proof (1/4)

Truth: X_t^1 with law $\overline{\psi}(t,x_1)dx_1$ and

$$\partial_t \overline{\psi} = \partial_1(\tilde{b}\overline{\psi}) + \partial_{1,1}\overline{\psi} \text{ where } \tilde{b}(t,x_1) = \frac{\displaystyle\int_{\mathbb{R}} \partial_1 V(x)\psi(t,x)dx_2}{\overline{\psi}(t,x_1)}.$$

Approximation: Z_t with law $\phi(t,x_1)dx_1$ and

$$\partial_t \phi = \partial_1(A'\phi) + \partial_{1,1}\phi \text{ where } A'(x_1) = \frac{\displaystyle\int_{\mathbb{R}} \partial_1 V(x)\psi_\infty(x)dx_2}{\overline{\psi_\infty}(x_1)}.$$

We would like to estimate $H\left(\overline{\psi}(t,\cdot)|\phi(t,\cdot)\right) = \displaystyle\int_{\mathbb{R}} \ln\left(\frac{\overline{\psi}}{\phi}\right)\overline{\psi}\,dx_1.$

Proof (2/4)

Step 1: Entropy estimate

One has

$$\partial_t \overline{\psi} = \partial_1(A'\overline{\psi}) + \partial_{1,1}\overline{\psi} + \partial_1((\tilde{b} - A')\overline{\psi})$$

and thus

$$\begin{aligned}
\frac{dH(\overline{\psi}|\phi)}{dt} &= -I(\overline{\psi}|\phi) + \int_{\mathbb{R}} \left(A' - \tilde{b}\right) \overline{\psi}\, \partial_1 \left(\ln \frac{\overline{\psi}}{\phi}\right) dx_1 \\
&\leq -I(\overline{\psi}|\phi) + \frac{1}{2}\int_{\mathbb{R}} \left(\partial_1 \left(\ln \frac{\overline{\psi}}{\phi}\right)\right)^2 \overline{\psi} + \frac{1}{2}\int_{\mathbb{R}} \left(A' - \tilde{b}\right)^2 \overline{\psi}\, dx_1 \\
&\leq \frac{1}{2}\int_{\mathbb{R}} \left(A' - \tilde{b}\right)^2 \overline{\psi}\, dx_1 .
\end{aligned}$$

Proof (3/4)

Step 2: Transport inequality [Grunewald/Otto/Villani/Westdickenberg]

For fixed t and x_1, let $\pi_t^{x_1}(dx_2, d\tilde{x}_2)$ be a coupling measure with marginals $\nu_t^{x_1} = \frac{\psi(t,x_1,x_2)}{\psi(t,x_1)}$ and $\nu_\infty^{x_1} = \frac{\psi_\infty(x_1,\tilde{x}_2)}{\psi_\infty(x_1,x_2)}$. We have, using (H2),

$$\left| A'(x_1) - \tilde{b}(t,x_1) \right| = \left| \int_{\mathbb{R}^2} \left(\partial_1 V(x_1,x_2) - \partial_1 V(x_1,\tilde{x}_2) \right) \pi_t^{x_1}(dx_2, d\tilde{x}_2) \right|$$
$$\leq \|\partial_{12} V\|_{L^\infty} \int_{\mathbb{R}^2} |x_2 - \tilde{x}_2| \, \pi_t^{x_1}(dx_2, d\tilde{x}_2).$$

Taking the infimum on $\pi_t^{x_1} \in \Pi\left(\nu_t^{x_1}, \nu_\infty^{x_1}\right)$,

$$\left| A'(x_1) - \tilde{b}(t,x_1) \right| \leq \|\partial_{12} V\|_{L^\infty} \; W_1(\nu_t^{x_1}, \nu_\infty^{x_1}).$$

We now use the Talagrand inequality and the LSI on $\nu_\infty^{x_1}$ (H1) to get

$$\left| A'(x_1) - \tilde{b}(t,x_1) \right| \leq \frac{\|\partial_{12} V\|_{L^\infty}}{\rho} \; \sqrt{I(\nu_t^{x_1} | \nu_\infty^{x_2})}$$

Proof (4/4)

Step 3: Conclusion

We thus have

$$\int_{\mathbb{R}} \left(A'(x_1) - \tilde{b}(t,x_1)\right)^2 \overline{\psi}(t,x_1)\,dx_1 \leq \frac{\|\partial_{12} V\|_{L^\infty}^2}{\rho^2} \int_{\mathbb{R}} I(\nu_t^{x_1} | \nu_\infty^{x_1}) \overline{\psi}$$
$$\leq \frac{\|\partial_{12} V\|_{L^\infty}^2}{\rho^2} I(\psi|\psi_\infty).$$

Plugging this into the entropy estimate, we get

$$\frac{dH(\overline{\psi}|\phi)}{dt} \leq \frac{\|\partial_{12} V\|_{L^\infty}^2}{2\rho^2} I(\psi|\psi_\infty)$$
$$= -\frac{\|\partial_{12} V\|_{L^\infty}^2}{2\rho^2} \frac{dH(\psi|\psi_\infty)}{dt}.$$

Integrating in time (since $H(\overline{\psi}(0,\cdot)|\phi(0,\cdot)) = 0$):

$$\forall t \geq 0,\ H(\overline{\psi}(t)|\phi(t)) \leq \frac{\|\partial_{12} V\|_{L^\infty}^2}{2\rho^2} \left(H(\psi(0)|\psi_\infty) - H(\psi(t)|\psi_\infty)\right).$$

Entropy techniques

Other results based on this set of assumptions (LSI for the conditional measures and bounded coupling):

- [TL, JFA 2008]
  LSI for the cond. meas. $\mu(\cdot|\xi(x)=z)$ + bdd coupling + LSI for the marginal $\xi * \mu \implies$ LSI for μ.
- [TL, Rousset, Stoltz Nonlinearity, 2008] Analysis of the adaptive biasing force method which writes, for $\xi(x_1,x_2)=x_1$:

$$\begin{cases} dX_t = -\nabla(V - A_t \circ \xi)(X_t)\,dt + \sqrt{2}dW_t\,, \\ A_t'(z) = \mathbb{E}(\partial_1 V(X_t)|\xi(X_t)=z). \end{cases}$$

Error analysis: trajectories

Theorem [Legoll, TL, Olla, 2017]

Let us recall that $\xi(x_1, x_2) = x_1$. Under the assumptions:

(H1') For all x_1, the conditional probability measures $\mu(\cdot|\xi(x) = x_1)$ satisfy a Poincaré inequality with constant ρ,

(H2') Bounded coupling assumption: $\|\partial_{12} V\|_{L^2(\mu)} \leq \kappa$,

(H3) b is one-sided Lipschitz ($-b' \leq L_b$) and such that
$$\int_{\mathbb{R}} \sup_{z\in[-|x_1|,|x_1|]} |b'(z)|^2 \overline{\mu}(dx_1) < \infty.$$

Then, if $Z_0 = \xi(X_0)$ is distributed according to a measure μ_0 such that $\frac{d\mu_0}{d\mu} \in L^\infty$,

$$\mathbb{E}\left(\sup_{t\in[0,T]} |\xi(X_t) - Z_t| \right) \leq C \frac{\kappa}{\rho}$$

The proof uses probabilistic arguments (Poisson equations and Doob's martingale inequalities).

Remark: Application to averaging principle

These techiques can be used to obtain quantitative results for averaging principles. For example, let us consider

$$\begin{cases} dX_t^{1,\varepsilon} = -\partial_1 V(X_t^\varepsilon)\,dt + \sqrt{2}dW_t^1 \\ dX_t^{2,\varepsilon} = -\dfrac{\partial_2 V(X_t^\varepsilon)}{\varepsilon}\,dt + \sqrt{\dfrac{2}{\varepsilon}}dW_t^2 \end{cases}$$

Then, under the assumptions above:

$$\mathbb{E}\left(\sup_{t\in[0,T]}\left|X_t^{1,\varepsilon} - Z_t\right|\right) \leq C\sqrt{\varepsilon}\,\frac{\kappa}{\rho}.$$

Recent extensions and on-going works

We recently extended these results to general vectorial reaction coordinates and to non-reversible dynamics (non-gradient forces) (collab. with U. Sharma and W. Zhang).

From a numerical viewpoint, these coarse-grained dynamics can be used as predictors in predictor-corrector schemes (parareal algorithms) (collab. with G. Samaey).

References

Review paper on multiscale models for polymeric fluids:

- C. Le Bris, TL, *Micro-macro models for viscoelastic fluids: modelling, mathematics and numerics*, Science China Mathematics, 2012.

Some papers I mentioned:

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- F. Legoll, TL and U. Sharma, *Effective dynamics for non-reversible stochastic differential equations: a quantitative study*, Nonlinearity, 2019.