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Optimal transport and dissipative systems Deterministic limits for stochastic processes

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Basic question

How does a dissipative system behave when placed in contact with a heat bath?

Aim

To use a time-incremental variational scheme to describe such systems as stochastic processes. Specifically, the variational scheme will arise as a perturbation/regularization of the deterministic variational set-up by an entropy-like term.

Main result

In the inertialess case, as time step $\downarrow 0$, we obtain deterministic gradient flows (with variational characterization).

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Backgro	und				

- R. Jordan, D. Kinderlehrer & F. Otto
 The variational formulation of the Fokker-Planck equation SIAM J. Math. Anal. 1998
- 🍆 K.

A phase-field model of dislocations in ductile single crystals Calif. Inst. of Technology 2003

O. & R. Radovitzky 1999, O. & E.A. Repetto 1999, O. &
 L. Stainier 1999... and many more



• Consider a (first order) dissipative system in \mathbb{R}^N as given by its equilibrium equations

$$\partial \Psi(\dot{x}) \ni - \operatorname{grad} E(t, x),$$

where

- E is an energetic potential, possibly time-dependent if there is some external loading ℓ ;
- Ψ is a dissipation potential.
- What happens when this system is placed in contact with a heat bath?
- Strategy: perturb/regularize the discrete-time variational formulation of the equilibrium equations.



- Time step h > 0; let $t_i := ih$.
- Work done moving along a "nice" path $\gamma \colon [t_i, t_{i+1}] \to \mathbb{R}^N$:

$$W(\gamma) := \underbrace{E(t_{i+1}, \gamma(t_{i+1})) - E(t_i, \gamma(t_i))}_{\text{energetic pot.}} + \underbrace{\int_{t_i}^{t_{i+1}} \Psi(\dot{\gamma}(t)) \, \mathrm{d}t}_{\text{dissipative pot.}}.$$

• Approximate the "work distance" $\inf_{\gamma} W(\gamma)$ by the incremental cost/work function

$$C(t_i, x_i, t_{i+1}, x_{i+1}) := E(t_{i+1}, x_{i+1}) - E(t_i, x_i) + (t_{i+1} - t_i)\Psi\left(\frac{x_{i+1} - x_i}{t_{i+1} - t_i}\right).$$

• Applying Euler-Lagrange to C gives the equilibrium equations.

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Heuristic definition

Given a time step h > 0, "temperature" parameter $\varepsilon > 0$ and cost function C, the *regularized optimal transport problem* is to find a joint probability density $u_{i+1}^{h,\varepsilon}(x_i, x_{i+1})$ on $(\mathbb{R}^N)^2$, with first marginal a given density $\rho_i^{h,\varepsilon}(x_i)$, minimizing

$$\begin{split} &\iint_{\mathbb{R}^N} C(x_i, x_{i+1}) u_{i+1}^{h,\varepsilon}(x_i, x_{i+1}) \\ &+ \varepsilon u_{i+1}^{h,\varepsilon}(x_i, x_{i+1}) \log u_{i+1}^{h,\varepsilon}(x_i, x_{i+1}) \, \mathrm{d} x_i \mathrm{d} x_{i+1}. \end{split}$$

Given a probability space $(\Omega, \mathscr{F}, \mathbb{P})$, the *regularized optimal* transport chain $X^{h,\varepsilon} \colon \mathbb{N}_0 \times \Omega \to \mathbb{R}^N$ is the Markov chain whose transition probabilities solve a causal sequence of such single-step problems. (!)



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Lemma

The single-step regularized optimal transport problem extends continuously from definition on $\mathcal{P}_{ac}(\mathbb{R}^N)$ to the space of all Radon measures on \mathbb{R}^N .

Lemma (cf., e.g. Jordan-Kinderlehrer '96)

A regularized optimal transport chain has transition probabilities $\mathbb{P}_{i+1}^{h,\varepsilon}(-|x_i)$ with densities $\rho_{i+1}^{h,\varepsilon}(-|x_i)$ with respect to Lebesgue measure given by

$$\rho_{i+1}^{h,\varepsilon}(x_{i+1}|x_i) = \frac{\exp\left(-\frac{1}{\varepsilon}C(x_i, x_{i+1})\right)}{\int_{\mathbb{R}^N} \exp\left(-\frac{1}{\varepsilon}C(x_i, x_{i+1})\right) \, \mathrm{d}x_{i+1}}.$$

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Definition

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Let $\bar{X}^{h,\varepsilon}: \Omega \times \mathbb{R}_{\geq 0} \to \mathbb{R}^N$ denote the continuous, piecewise affine interpolation

$$\bar{X}_t^{h,\varepsilon} := X_{\lfloor t/h \rfloor}^{h,\varepsilon} + \left(\frac{t}{h} - \left\lfloor \frac{t}{h} \right\rfloor\right) \left(X_{\lfloor t/h \rfloor+1}^{h,\varepsilon} - X_{\lfloor t/h \rfloor}^{h,\varepsilon}\right)$$

Thus, $\bar{X}^{h,\varepsilon}$ is a measurable function (random variable)

$$\bar{X}^{h,\varepsilon} \colon \Omega \to C^0(\mathbb{R}_{\geq 0}; \mathbb{R}^N),$$

and we can consider the law (push-forward measure) $(ar{X}^{h,arepsilon})_{..}(\mathbb{P})$ on the space of continuous paths in \mathbb{R}^N , take (weak) limits as $h \downarrow 0 \& c.$



- Get as much information as we can about the transition densities $\rho_{i+1}^{h,\varepsilon}(-|x_i)$.
- Hope that the increments follow some "decent" distribution

$$\Delta X_{i+1}^{h,\varepsilon} \equiv X_{i+1}^{h,\varepsilon} - X_i^{h,\varepsilon} \sim \text{Distrib}\left(X_i^{h,\varepsilon}, h, \varepsilon, E, \Psi\right).$$

 Apply a central limit theorem to say something about the distribution of the continuous-time increments as h ↓ 0:

$$\bar{X}_{t}^{h,\varepsilon} - \bar{X}_{s}^{h,\varepsilon} \approx X_{\lfloor t/h \rfloor}^{h,\varepsilon} - X_{\lfloor s/h \rfloor}^{h,\varepsilon} = \sum_{i=\lfloor s/h \rfloor}^{\lfloor t/h \rfloor - 1} \Delta X_{i+1}^{h,\varepsilon} \xrightarrow[h\downarrow 0]{} \operatorname{Normal}(?,?).$$

 Conclude something interesting about the limiting measure on path space.



Relationship with noise

Why should this optimal transport scheme be considered a valid model for $\partial \Psi(\dot{x}) \ni - \operatorname{grad} E(t, x) +$ "noise"?

"Proof by example" (linear kinetics and Ito diffusions)

On \mathbb{R}^N , consider:

- a coercive, C^2 energetic potential $E \colon \mathbb{R}^N \to \mathbb{R}$;
- a viscous (i.e. 2-homogeneous), isotropic dissipative potential $\Psi : \mathbb{R}^N \to \mathbb{R}, \Psi(\dot{x}) := \frac{1}{2} |\dot{x}|^2.$

The key observation about the increments is that

$$X_{i+1}^{h,\varepsilon} - X_i^{h,\varepsilon} \sim \operatorname{Normal}\left(-\frac{h}{2}\operatorname{grad} E(X_i^{h,\varepsilon}), \varepsilon h\right)$$



Theorem (cf. Jordan-Kinderlehrer-Otto '98)

Given $\varepsilon > 0$, let $X^{h,\varepsilon}$ be the optimal transport chain for the potentials on the previous slide starting at $x_0 \in \mathbb{R}^N$. Then

$$\bar{X}^{h,\varepsilon} \xrightarrow[h\downarrow 0]{} Y^{\varepsilon},$$

where

$$\begin{cases} \dot{Y}_t^{\varepsilon} = -\operatorname{grad} E(Y_t^{\varepsilon}) + \sqrt{\varepsilon} \dot{W}_t; \\ Y_0^{\varepsilon} = x_0. \end{cases}$$

 $\textit{I.e. } \mathbb{P}\big[\bar{X}^{h,\varepsilon} \in B\big] \xrightarrow[h\downarrow 0]{} \mathbb{P}[Y^{\varepsilon} \in B] \textit{ for all Borel } B \subseteq C^0\big(\mathbb{R}_{\geq 0}; \mathbb{R}^N\big).$



Consider the following toy model for an inertialess slider subject to time-dependent loading ℓ , dissipation Ψ and a heat bath with "temperature" ε :

• time-dependent energetic potential $E(t,x) = -\ell(t) \cdot x$;

• Lipschitz forcing/loading $\ell \colon [0,T] \to \mathbb{R}^N$;

• 1-homogeneous, positive-definite dissipative potential $\Psi \colon \mathbb{R}^N \to [0, +\infty);$

• e.g. isotropic case $\Psi(\dot{x}) = \sigma |\dot{x}|;$

• More generally, call $\sigma := \min_{|\dot{x}|=1} \Psi(\dot{x})$ the critical load. Consider loadings ℓ with $\|\ell\|_{C^0} < \sigma$.

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- Consider the increment $\Delta X_{i+1}^{h,\varepsilon}\equiv X_{i+1}^{h,\varepsilon}-X_{i}^{h,\varepsilon}.$
- The mean scales like ε , but the variance scales like ε^2 , and both are independent of h:

$$\mathbb{E}\left[\Delta X_{i+1}^{h,\varepsilon} \middle| X_i^{h,\varepsilon}\right] = \mathbb{E}\left[\Delta X_{i+1}^{h,\varepsilon}\right] = \varepsilon \xi_{\text{eff}}(t_{i+1});$$

$$\operatorname{Var}\left[\Delta X_{i+1}^{h,\varepsilon} \middle| X_i^{h,\varepsilon}\right] = \operatorname{Var}\left[\Delta X_{i+1}^{h,\varepsilon}\right] \le \operatorname{const} \cdot \varepsilon^2;$$

where the *effective load/drift* is

$$\xi_{\text{eff}}(t_{i+1}) = \frac{\int_{\mathbb{R}^N} z \exp\left(z \cdot \ell(t_{i+1}) - \Psi(z)\right) dz}{\int_{\mathbb{R}^N} \exp\left(z \cdot \ell(t_{i+1}) - \Psi(z)\right) dz}$$

• Ignoring the variance part, this looks rather like an Euler approximation for the ODE $\dot{Y}_t = \xi_{\text{eff}}(t)$ with time step ε .

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Definition

An effective kinetic potential for $\xi_{\rm eff}$ is given by

$$\varphi_{\text{eff}}(t, x) = -\xi_{\text{eff}}(t) \cdot x.$$

In the isotropic case $\Psi(\dot{x})=\sigma|\dot{x}|$ (K. '03),

- ΔX_{i+1} is a Laplace random variable;
- the effective load is

$$\xi_{\text{eff}}(t) = \frac{(N+1)\ell(t)}{\sigma^2 - |\ell(t)|^2};$$

• the effective kinetic potential is

$$\varphi_{\text{eff}}(t,x) = -\frac{(N+1)\ell(t) \cdot x}{\sigma^2 - |\ell(t)|^2}.$$



- It sits well with comparison with the implicit Euler scheme.
- Dimensionally, this corresponds to energy input at power ε/h .
- Alternatively, if one were to naïvely apply the central limit theorem:

$$\bar{X}_{t}^{h,\varepsilon} - x_{0} \approx X_{\lfloor t/h \rfloor}^{h,\varepsilon} - x_{0} = \sum_{i=0}^{\lfloor t/h \rfloor - 1} \Delta X_{i+1}^{h,\varepsilon}$$
$$\sim \operatorname{Normal}\left(\sum_{i=0}^{\lfloor t/h \rfloor - 1} \mathbb{E}[\Delta X_{i+1}^{h,\varepsilon}], \sum_{i=0}^{\lfloor t/h \rfloor - 1} \operatorname{Var}[\Delta X_{i+1}^{h,\varepsilon}]\right)$$

but, as $h \downarrow 0$, a sum of $\lfloor t/h \rfloor$ terms of order ε

- diverges if ε is of order $h^p\text{, }p<1\text{;}$
- converges to 0 if ε is of order $h^p, \ p>1.$



Theorem (K.-O.-S.-T. '07)

For $\ell \in C^{0,1}([0,T];\mathbb{R}^N)$ with $\|\ell\|_{C^0} < \sigma$ and $\theta > 0$, let $Y^{\theta} : [0,T] \to \mathbb{R}^N$ solve the deterministic IVP

$$\begin{cases} \dot{Y}_t^{\theta} = \theta \xi_{\text{eff}}(t) \equiv -\theta \operatorname{grad} \varphi_{\text{eff}}(t, Y_t^{\theta}); \\ Y_0^{\theta} = x_0. \end{cases}$$

Then, for $\lambda > 0$, taking $\varepsilon = \theta h$,

$$\mathbb{P}\left[\left\|\bar{X}^{h,\theta h} - Y^{\theta}\right\|_{C^{0}}^{2} \ge \lambda\right] \le \frac{\operatorname{const} \cdot \theta^{2} T h}{\lambda^{2}},$$

I.e., $\bar{X}^{h,\theta h} \to Y^{\theta}$ in probability (and hence in law) in path space $C^0([0,T];\mathbb{R}^N)$ (with the supremum norm).



Corollary (via Brézis-Ekeland principle)

For $\ell \in C^{0,1}([0,T];\mathbb{R}^N)$ with $\|\ell\|_{C^0} < \sigma$ and $\theta > 0$,

$$\bar{X}^{h,\theta h} \xrightarrow[h\downarrow 0]{\mathbb{P}} Y^{\theta} \text{ in } C^0([0,T];\mathbb{R}^N),$$

where Y^{θ} is the unique minimizer of the action functional ${\mathscr S}$ given by

$$\mathscr{S}[Y] := \int_0^T \mathscr{L}(t, Y_t, \dot{Y}_t) \, \mathrm{d}t,$$
$$\mathscr{L}(t, x, v) := \frac{1}{2} |v - \theta \xi_{\mathrm{eff}}(t)|^2.$$





- $Y_t = \frac{\text{length}}{\text{ref.length}}$ for a material sample subjected to constant load $\ell \ll$ yield stress of the material.
- Linear strain hardening:

$$\sigma = \sigma_0 Y.$$

• For ℓ small in comparison to σ ,

$$\dot{Y}_t = \frac{2\theta\ell}{\sigma_0^2 Y_t^2 - \ell^2} \approx \frac{2\theta\ell}{\sigma_0^2 Y_t^2}.$$

- \rightsquigarrow Andrade's creep law: strain grows like $t^{1/3}$.
- Hardening exponent $\beta \rightsquigarrow$ creep exponent $1+2\beta.$





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 Orry friction in a parabolic energetic landscape

Consider the the following toy model for an inertialess gradient flow in E subject to dissipation Ψ and a heat bath with "temperature" ε

- energetic potential: $E(t,x) := \frac{1}{2}x \cdot Ax \ell(t) \cdot x$ with A = Hess(E) symmetric and positive-definite;
- dissipative potential: $\Psi : \mathbb{R}^N \to \mathbb{R}$ 1-homogeneous with critical load $\sigma = \min_{|\dot{x}|=1} \Psi(\dot{x}) > 0$;

• "interesting" / admissible region B,

$$\mathcal{B}(\ell(t)) = \left\{ x \in \mathbb{R}^N \big| |\ell(t) - Ax| < \sigma \right\}$$
$$= A^{-1}\ell(t) + A^{-1}\mathbb{B}_{\sigma}(0).$$

I.e., the previous model with the slider restrained by a spring with elasticity matrix A.



For each $x_i \in \mathbb{R}^N$, the transition density $\rho_{i+1}^{h,\varepsilon}(-|x_i)$ is unimodal: the mode is precisely the (unique) closest point of $\overline{\mathcal{B}(\ell(t_{i+1}))}$ to x_i .



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• Same ε - ε^2 scaling for mean and variance of $\Delta X_{i+1}^{h,\varepsilon}$, but the effective load is no longer independent of ε or prior position. For $X_i^{h,\varepsilon} \in \mathcal{B}(\ell(t_{i+1}))$,

$$\mathbb{E}\left[\Delta X_{i+1}^{h,\varepsilon} \middle| X_i^{h,\varepsilon}\right] = \varepsilon \xi^{\varepsilon} \big(t_{i+1}, X_i^{h,\varepsilon}\big);$$

$$\operatorname{Var}\left[\Delta X_{i+1}^{h,\varepsilon} \middle| X_i^{h,\varepsilon}\right] \le \frac{\operatorname{const}}{\left(\sigma^2 - \left|\ell(t_{i+1}) - AX_i^{h,\varepsilon}\right|^2\right)^2} \varepsilon^2 + o(\varepsilon^2);$$

where

$$\xi^{\varepsilon}(t,x) := \frac{\int_{\mathbb{R}^N} z \exp\left(-\left(z \cdot (Ax - \ell(t)) + \Psi(z) + \frac{\varepsilon}{2}z \cdot Az\right)\right) \, \mathrm{d}z}{\int_{\mathbb{R}^N} \exp\left(-\left(z \cdot (Ax - \ell(t)) + \Psi(z) + \frac{\varepsilon}{2}z \cdot Az\right)\right) \, \mathrm{d}z}$$

• Given $X_i \notin \overline{\mathcal{B}}$, $X_{i+1}^{h,\varepsilon}$ has mean the nearest point of $\partial \mathcal{B}$ and variance of order ε .

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Effective	gradie	nt structure			

Lemma

For $\varepsilon \geq 0, \, A$ symmetric and positive-definite, $\xi^{\varepsilon}(t,x)$ is the gradient in x of

$$\varphi^{\varepsilon}(t,x) := \log \int_{\mathbb{R}^N} \exp\left(-\left(z \cdot (Ax - \ell(t)) + \Psi(z) + \frac{\varepsilon}{2}z \cdot Az\right)\right) \, \mathrm{d}z,$$

with respect to the the constant Riemannian metric A, i.e.

$$\xi^{\varepsilon}(t,x) = -\operatorname{grad}_A \varphi^{\varepsilon}(t,x) \equiv -A^{-1} \mathrm{d} \varphi^{\varepsilon}(t,x).$$

Definition

As before, call $\xi_{eff} := \xi^0$ the effective load and $\varphi_{eff} := \varphi^0$ the effective kinetic potential.

In the isotropic case $\Psi(\dot{x})=\sigma|\dot{x}|,$

• the effective load is

$$\xi_{\rm eff}(t,x) = \frac{(N+1)(\ell(t) - Ax)}{\sigma^2 - |\ell(t) - Ax|^2};$$

• the effective kinetic potential is

$$\varphi_{\text{eff}}(t,x) = -\frac{N+1}{2} \log \left(\sigma^2 - |\ell(t) - Ax|^2\right);$$

and

$$\xi_{\rm eff}(t,x) = -\operatorname{grad}_A \varphi_{\rm eff}(t,x) \equiv -A^{-1} \mathrm{d}\varphi_{\rm eff}(t,x).$$





The effective potential φ_{eff} in dimensions N = 1, 2 for $\ell(t) = 0$, $\Psi(\dot{x}) = \sigma |\dot{x}|$. Note the blow-up at the boundary of the "admissible region", i.e. where net force equals dissipation.

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Theorem (K.-O.-S.-T. '07)

Let $\theta > 0$; let $Y^{\theta} \colon [0,T] \to \mathbb{R}^N$ solve the deterministic IVP

$$\begin{cases} \dot{Y}_t^{\theta} = \theta \xi_{\text{eff}}(t, Y_t^{\theta}) \equiv -\theta \operatorname{grad}_A \varphi_{\text{eff}}(t, Y_t^{\theta}); \\ Y_0^{\theta} = x_0 \in \mathcal{B}(\ell(0)); \end{cases}$$

Then, for $\lambda > 0$, taking $\varepsilon = \theta h$,

$$\mathbb{P}\left[\left\|\bar{X}^{h,\theta h} - Y^{\theta}\right\|_{C^{0}}^{2} \ge \lambda\right] \in O(h) \text{ as } h \downarrow 0.$$

I.e., $\bar{X}^{h,\theta h} \to Y^{\theta}$ in probability (and hence in law) in path space $C^0([0,T];\mathbb{R}^N)$ (with the supremum norm).



Corollary

With the same assumptions as before,

$$\bar{X}^{h,\theta h} \xrightarrow[h\downarrow 0]{\mathbb{P}} Y^{\theta} \text{ in } C^0([0,T];\mathbb{R}^N),$$

where Y^{θ} is the unique minimizer of the action functional ${\mathscr S}$ given by

$$\mathscr{S}[Y] := \int_0^T \mathscr{L}(t, Y_t, \dot{Y}_t) \, \mathrm{d}t,$$
$$\mathscr{L}(t, x, v) := \frac{1}{2} |v - \theta \xi_{\mathrm{eff}}(t, x)|^2.$$





Comparison of the limiting gradient flow $\dot{Y}_t = -\varphi'_{\text{eff}}(Y_t)$ (black) with the "frictionless" gradient flow $\dot{Z}_t = -AZ_t$ (red).





 Y_t^{θ} in greyscale. From darkest to lightest: $\theta = 0, 1, 2, 10, 50$. $\theta = 0 \leftrightarrow$ rate-independent limit at zero temperature.





In black, the "yield surface" $\partial \mathcal{B} = \sigma A^{-1}(\mathbb{S}^1)$. In colour, trajectories for $Y_t, t \in [0, 100]$, for various initial data. Note the approach along the eigenvector of A^{-1} with largest eigenvalue.



In black, the "yield surface" $\partial \mathcal{B} = \sigma A^{-1}(\mathbb{S}^1)$. In colour, trajectories for $Y_t, t \in [0, 100]$, for various initial data. Note the approach along the eigenvector of A^{-1} with largest eigenvalue.

-1

.25

-0.5

-0.75



- The optimal transport scheme can describe stochastic processes such as Itō diffusions.
- It can also describe dry-friction-like systems, at least when inertia is neglected.
- We extract a deterministic limit (with gradient structure and minimum principle) from an *a priori* stochastic system by exploiting the dependence of the regularization parameter on the length of then time step.
- The resulting evolutions encompass physical processes such as creep.

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- How is $\theta = \frac{\varepsilon}{h}$ related to physical temperature?
- Energies with positive-*semi*-definite and/or non-constant Hessian *A*?
- Incorporation of inertial effects?
 - Heated harmonic oscillators? Belt friction?
 - Other slipping processes, e.g. earthquakes, fluid invasion & c.?
- Can the analysis be extended to infinite-dimensional and/or curved state spaces and make better use of the general set-up for optimal transport chains?

Main point

Despite connections with steepest descent methods, the optimal transport framework is somewhat *ad hoc*: can it be justified e.g. from wiggly energies with stochastic noise?

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Theorem (Abeyaratne-Chu-James '96; S.-T. '07)

For a "decent" potential $V \colon \mathbb{R} \to \mathbb{R}$, let X^{ε} satisfy the forced wiggly gradient flow

$$\dot{X}^{\varepsilon}(t) = -V'(X^{\varepsilon}(t)) - g\left(\frac{X^{\varepsilon}(t)}{\varepsilon}\right) + \ell(\varepsilon t).$$

Then $X^0(t) := \lim_{\varepsilon \downarrow 0} X^{\varepsilon}(t/\varepsilon)$ satisfies the inclusion

$$\partial \left| \dot{X}^0(t) \right| \ni -V' \left(X^0(t) \right) + \ell(t)$$

iff $g: \mathbb{R} \to [-1,1]$ attains its bounds "often enough" (e.g. periodic [A.-C.-J.], or almost any sample path of doubly reflected Brownian motion [S.-T.]).

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Conjecture/Hope

For "decent" potentials V, perturbations g and the right scaling $\sigma=\sigma(\varepsilon),$ solutions of

$$\dot{X}^{\varepsilon}(t) = -V'\left(X^{\varepsilon}(t)\right) - g\left(\frac{X^{\varepsilon}(t)}{\varepsilon}\right) + \ell(t) + \sigma(\varepsilon)\dot{W}(t)$$

converge as $\varepsilon \downarrow 0$ to the trajectory predicted by the optimal transport chain method — noise "activates" the system in a deterministic way in the admissible (sticking) region.