Scale-bridging for entropic flows in the presence of energy or noise

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Support: ITN Fronts and InteRfaces in Science and Technology, EPSRC, Leverhulme

Overdamped Langevin: entropic gradient flows

Particles and deterministic gradient flows

From particles to diffusion

Brownian motion (Pollen grains in fluid, R. Brown 1827)

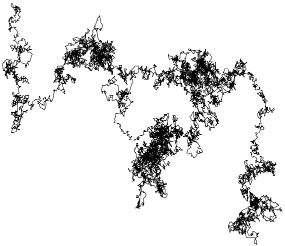


Figure : Brownian motion, taken from Mörters & Peres, *Brownian Motion*

Macroscopic (many-particle) limit:
Let $\rho = \rho(x,t)$ be the particle density (number of particles per unit volume) at position x and time t. Then ρ satisfies the diffusion equation,

$$\frac{\partial}{\partial t}\rho(x,t) = \Delta\rho(x,t)$$
$$= \mathrm{div}\left(\rho(x,t)\nabla\frac{\delta \mathsf{S}}{\delta\rho}(\rho)\right) = \mathsf{K}\,\mathrm{d}\mathsf{S} \quad (1)$$

(*"Wasserstein flow"*) with entropy $\mathsf{S}(\rho) := \int_{\mathbb{R}^n}\rho(x)\log\rho(x)\,\mathrm{d}x$.

Question: How can we *derive (1) and stochastic "corrections" directly from particles?* (e.g., helpful in nonlinear case, with potential,. . .)

What is a large deviation principle? An example

Sanov's theorem

In *equilibrium* (static situation):
Let X_i $(i = 1, 2, \dots)$ be independent and identically distributed stochastic variables with distribution μ on a state space X (positions of particles)
Their concentration is given by the *empirical measure* $\rho_n := \frac{1}{n}\sum_{i=1}^n \delta_{X_i}$.
Sanov's theorem states: the random measure ρ_n satisfies the *large-deviation principle*

$$\mathrm{Prob}(\rho_n \approx \rho) \sim \exp[-nJ(\rho)], \qquad \text{as } n \to \infty, \tag{2}$$

where the *rate function* $I \geq 0$ is the *relative entropy* of ρ with respect to μ,

$$J(\rho) = H(\rho|\mu) := \begin{cases} \int f \log f \, d\mu & \text{if } \rho \ll \mu \text{ and } \rho = f\mu, \\ +\infty & \text{otherwise.} \end{cases}$$

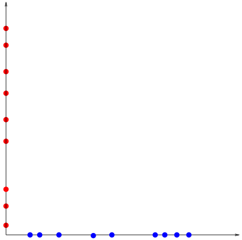
See Touchette, *Phys. Rep.*, **478** (2009), 1 for an excellent review of large deviations and thermodynamics.

Dynamics: The microscopic picture

Particle model

Brownian motion: the probability that a particle jumps in time $h > 0$ from $x \in \mathbb{R}$ to $y \in \mathbb{R}$ is $p_h(x, y) := \frac{1}{2\sqrt{\pi h}} \exp(-(y-x)^2/4h)$.

Possible particle jumps:



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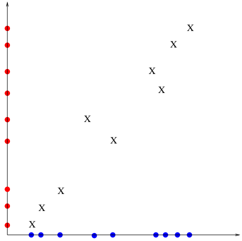

Every blue particle has to jump to a red one (be identified with a red one)

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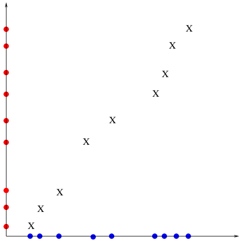

Jumps maximise $\Pi \exp(-(x_i - y_i)^2/(4h)) = \exp^{-\sum (x_i - y_i)^2/(4h)}$, yields cost functional $(x-y)^2$ of Wasserstein metric $d(\rho_0, \rho_1)^2 :=$

$$\inf_{\substack{\gamma \,\mid\, \gamma(A, \mathbb{R}^n) = \rho_0(A), \\ \gamma(\mathbb{R}^n, A) = \rho_1(A)}} \int_{\mathbb{R}^n \times \mathbb{R}^n} (x-y)^2 \, \gamma(dxdy).$$

(Léonard 2007, Gozlan, Léonard, *Prob. Th. Rel. Fields*, **139** (2007), 235–283; Adams, Dirr, Peletier, Zimmer, *Comm. Math. Phys.*, **307** (2011), 791–815; Dirr, Laschos, Zimmer, *J. Math. Phys.*, **53** (2012), 063704)

Large deviations: from particles to PDEs

Dawson-Gärtner theorem

Given n Brownian particles and a fixed terminal time $T > 0$, consider the path of *empirical measures* $[0, T] \ni t \mapsto \rho_n(t) = \frac{1}{n}\sum_{j=1}^{n} \delta_{X(j)}$.
Then (Dawson, Gärtner, *Mem. Amer. Math. Soc.*, **78** (1989); Kipnis, Olla, *Stochastics Rep.*, **33** (1990), 17–25):

$$\mathrm{Prob}(\rho_n \approx \rho) \sim \exp[-nJ(\rho)], \tag{3}$$

with the *rate functional* (norms defined on next slide)

$$J(\rho) := \frac{1}{2}\int_0^T \left\| \frac{\partial \rho}{\partial t} - \Delta\rho \right\|_{\rho(t),*}^2 \mathrm{d}t \tag{4}$$

See Touchette, *Phys. Rep.*, **478** (2009), 1 for large deviations and thermodynamics.

- Limit particle number $n \to \infty$: (3) gives vanishing probability to all states ρ except those for which $J(\rho) = 0$, the solution of the heat equation. (wiggly / multiwell potential: Dupuis, Spiliopoulos, *Stochastic Process. Appl.*, **122** (2012), 1947–1987)

Towards a stochastic PDE

Interpretation of the Dawson-Gärtner large deviation principle

A deterministic PDE, the heat equation, appears as minimiser of the rate function. The rate functional contains more information, though, such as on microscopic fluctuations.

Question: *How to obtain "stochastic corrections" to the heat equation, capturing such fluctuations in a systematic manner?*

Three ways to think about noisy variants of the heat equation

Possible questions:

1. Which noise is compatible with the Wasserstein geometry?
2. How can a noise term be derived from a particle model?
3. Is there a stochastic equation that yields in a limit the Dawson-Gärtner rate functional?

All three questions lead to *equations of fluctuation hydrodynamics* ("*Dean's equation*", Dean, *J. Phys. A: Math. Gen.*, **29** (1996), L613–L617)

$$\frac{\partial \rho}{\partial t} = \Delta \rho + \operatorname{div}(\sqrt{\rho} W) \tag{5}$$

with space-time white noise $W := W(x,t) := W_{x,t}$.

Dean's equation

Dean's derivation (with on-site potential)

Consider n particles governed by

$$dX_t^j = -\nabla V(X_t^j)dt + dB_t^j, \quad j = 1, \ldots, n$$

with potential V and n independent Brownian motions B_t^j. Let $\rho^j(x,t) := \delta(x - X_t^j)$ for $j = 1, \ldots, n$ and $\rho(x,t) := \sum_{j=1}^n \rho^j(x,t)$.

Step 1. A standard (Itō) calculation yields ($W_t dt = dB_t$)

$$\frac{\partial}{\partial t}\rho(x,t) = \frac{1}{2}\Delta\rho(x,t) + \operatorname{div}\left(\rho(x,t)\nabla V(x)\right) - \sum_{j=1}^n \operatorname{div}(\rho^j(x,t)W_t^j).$$

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Step 2. A miracle occurs: replace noise term to get closed form.
Step 3. Result: Dean's equation

$$\frac{\partial}{\partial t}\rho(x,t) = \frac{1}{2}\Delta\rho(x,t) + \operatorname{div}(\sqrt{\rho(x,t)}W(x,t)).$$

More explicit in step 2

Key idea in Dean's derivation

Noise

$$\xi(x,t) := \sum_{j=1}^{n} \mathrm{div}(\rho^j(x,t) W_t^j). \tag{6}$$

is not closed (depends on ρ^j rather than ρ).
Replace this noise by another one with the same statistical properties.

Lemma

Interpreted in a distributional sense, $\xi(x,t)$ is a centred Gaussian process.

Define the "Dean noise" $\zeta(x,t)$ as the generalised process

$$\zeta(x,t) := \mathrm{div}\left(\sqrt{\rho(x,t)}W(x,t)\right).$$

Lemma

The generalised processes $\zeta(x,t)$ and $\xi(x,t)$ are equal in distribution (have the same characteristic function).

Dean's equation and large deviations

Dean's equation and Wasserstein geometry

1. Particle model led to Dean's equation, and this noise is compatible with the Wasserstein geometry (von Renesse and Sturm, *Ann. Probab.*, **37** (2009), 1114–1191). Why?
2. Can Dean's equation be related to diffusion equation by large deviation principle?

Formal large deviation analysis

Consider *scaled* Dean's equation (vanishing noise $h \to 0$):

$$\frac{\partial}{\partial t}\rho(x,t) = 1\cdot\Delta\rho(x,t) + h\,\mathrm{div}(\sqrt{\rho(x,t)}W(x,t)).$$

From fluctuating hydrodynamics to Wasserstein geometry

Tailleur, Kurchan, Lecomte, *J. Phys. A*, **41** (505001), 2008: For (scaled) fluctuating hydrodynamics,

$$\frac{\partial}{\partial t}\rho(x,t) = 1\cdot\Delta\rho(x,t) + h\,\mathrm{div}(\sqrt{\rho(x,t)}W(x,t)).$$

most likely path maximiser of (a path integral)

$$\int\int \exp\left(-\frac{1}{h^2}\int\int\left[\hat\rho\partial_t\rho + \nabla\rho\cdot\nabla\hat\rho - \rho|\nabla\hat\rho|^2\,\mathrm{d}x\,\mathrm{d}t\right]\right)\mathcal{D}\rho\mathcal{D}\hat\rho. \qquad (7)$$

Eliminate $\hat\rho$: its Euler-Lagrange equation is $\partial_t\rho = [\Delta\rho - 2\nabla\cdot(\rho\nabla\hat\rho)]$. Use Wasserstein geometry: $\Delta\rho = \mathrm{div}(\rho\nabla\frac{\delta}{\delta\rho}S[\rho])$, for entropy $S[\rho] = \int_{\mathbb{R}^n}\rho(x)\log\rho(x)\,\mathrm{d}x$. Hence optimal $\hat\rho^* = \frac{1}{2}\left(\frac{\delta}{\delta\rho}S[\rho] - \Phi\right)$, where Φ solves $\partial_t\rho = \nabla\cdot(\rho D\nabla\Phi)$. Substitute back in (7). Result: maximisation over

$$-\frac{1}{4h^2}\int\int\rho\left|\nabla\left(\Phi - \frac{\delta}{\delta\rho}S[\rho]\right)\right|^2\mathrm{d}x\,\mathrm{d}t = -\frac{1}{4h^2}\int_0^T\left\|\frac{\partial\rho}{\partial t} - \Delta\rho\right\|^2_{\rho(t),*}\mathrm{d}t. \qquad (8)$$

So *we obtain in the limit not only the deterministic PDE, but the rate functional (which describes in addition fluctuations around minimum)*.

Summary of the last arguments

What have we learnt?

1. Limit of vanishing noise: one expects to recover the associated deterministic PDE. Dean's equation is special since this noise does more: it recovers in the limit the associated *rate functional* (Dawson-Gärtner, or Jordan-Kinderlehrer-Otto), and hence the metric structure.
2. This explains link between Dean's particle derivation and the analysis of von Renesse and Sturm (*"Wasserstein-compatible noise"*, von Renesse and Sturm, *Ann. Probab.*, **37** (2009), 1114–1191; Andres and von Renesse, *J. Funct. Anal.*, **258** (2010), 3879–3905). (Joint work with Rob Jack)

What have we not (yet) learnt?

1. Matheatical analysis à la Tailleur *et al.*
2. Is this approach general, connecting particle models / stochastic equations to (geo-)metric formulations of PDE?

Second order Langevin equation & GENERIC

General nonequilibrium equations

Nonequilibrium framework (GENERIC)

General Equation for Non-Equilibrium Reversible-Irreversible Coupling
(H.-Ch. Öttinger, Beyond Equilibrium Thermodynamics, Wiley, 2005)

$$\partial_t z = \mathsf{L}(z)\,\mathsf{dE}(z) + \mathsf{K}(z)\,\mathsf{dS}(z), \tag{9}$$

- $\mathsf{E}, \mathsf{S} \colon Z \to \mathbb{R}$ are the energy and entropy functionals,
- dE, dS are appropriate derivatives (Fréchet derivative or a gradient with respect to some inner product);
- $\mathsf{L} = \mathsf{L}(z)$ is an antisymmetric operator satisfying the Jacobi identity

  $$\{\{\mathsf{F}_1, \mathsf{F}_2\}_\mathsf{L}, \mathsf{F}_3\}_\mathsf{L} + \{\{\mathsf{F}_2, \mathsf{F}_3\}_\mathsf{L}, \mathsf{F}_1\}_\mathsf{L} + \{\{\mathsf{F}_3, \mathsf{F}_1\}_\mathsf{L}, \mathsf{F}_2\}_\mathsf{L} = 0$$

  for all functions $\mathsf{F}_i \colon Z \colon Z \to \mathbb{R},$, with Poisson bracket $\{\cdot,\cdot\}_\mathsf{L}$

  $$\{\mathsf{F}, \mathsf{G}\}_\mathsf{L} := \mathsf{dF} \cdot \mathsf{L}\,\mathsf{dG}$$

- $\mathsf{K} = \mathsf{K}(z)$ is symmetric and positive semidefinite.

General nonequilibrium equations

Nonequilibrium framework (GENERIC)

The building blocks $\{\mathsf{L}, \mathsf{K}, \mathsf{E}, \mathsf{S}\}$ are required to fulfil the *degeneracy conditions*: for all $z \in Z$,

$$\mathsf{L}\,\mathsf{dS} = 0, \quad \mathsf{K}\,\mathsf{dE} = 0. \tag{10}$$

As a consequence, energy is conserved along a solution, and entropy is non-decreasing:

$$\frac{d\mathsf{E}(z(t))}{dt} = \mathsf{dE} \cdot \frac{dz}{dt} = \mathsf{dE} \cdot (\mathsf{L}\,\mathsf{dE} + \mathsf{K}\,\mathsf{dS}) = 0,$$
$$\frac{d\mathsf{S}(z(t))}{dt} = \mathsf{dS} \cdot \frac{dz}{dt} = \mathsf{dS} \cdot (\mathsf{L}\,\mathsf{dE} + \mathsf{K}\,\mathsf{dS}) = \mathsf{dS} \cdot \mathsf{K}\,\mathsf{dS} \geq 0.$$

A GENERIC system is then fully characterised by $\{Z, \mathsf{E}, \mathsf{S}, \mathsf{L}, \mathsf{K}\}$.

GENERIC

Use so far

- Öttinger and group: formal scale-bridging from microscopic Hamiltonian models to GENERIC as continuum description
- Thermodynamic consistent modelling (fluids, quantum systems coupled to macroscopic dissipative ones, elastoplasticity, . . . : e.g., Mielke, *Contin. Mech. Thermodyn.*, **23** (2011), 233–256)

Current questions

- Can we derive simple GENERIC systems rigorously from mesoscopic models?
- Analysis for GENERIC systems (existence / time splitting methods, . . .).

Motion with inertia

Vlasov-Fokker-Planck equation

Duong, Peletier, Z.: Revisit Vlasov-Fokker-Planck equation in light of GENERIC equation (9), $\rho = \rho(q, p)$.

$$\partial_t \rho = -\mathrm{div}_q\Big(\rho \frac{p}{m}\Big) + \mathrm{div}_p \rho\Big(\nabla_q V + \nabla_q \psi * \rho + \gamma \frac{p}{m}\Big) + \gamma\theta\Delta_p \rho. \quad (11)$$

This is many particle limit of *interacting Brownian particles with inertia*,

$$\begin{aligned} dQ_i(t) &= \frac{P_i(t)}{m}\, dt, \\ dP_i(t) &= -\nabla V(Q_i(t))\, dt - \sum_{j=1}^{n} \nabla\psi(Q_i(t) - Q_j(t)) \\ &\quad - \frac{\gamma}{m} P_i(t)\, dt + \sqrt{2\gamma\theta}\, dB_i(t) \end{aligned}$$

(Q_i and P_i position and momentum of particle $i = 1, \ldots, n$, mass m, potential V, interaction potential ψ, drift term $-\gamma P_i dt/m$, stochastic forcing by n independent Wiener measures B_i).

Vlasov-Fokker-Planck equation as GENERIC equation

Microscopic energy balance

The VFP equation (11) is *not* of GENERIC form: there is no conserved functional E. Physical reason: Particle model from last slide has heat bath interaction, which affects natural Hamiltonian

$$H_n(Q_1,\dots,Q_n,P_1,\dots,P_n) := \frac{1}{n}\sum_{i=1}^{n}\left[\frac{P_i^2}{2m}+V(Q_i)\right]+\frac{1}{2n^2}\sum_{i,j=1}^{n}\psi(Q_i-Q_j);$$

a calculation shows $dH_n = -\frac{1}{n}\sum_{i=1}^{n}\left[\frac{\gamma}{m^2}P_i^2\,dt - \frac{\gamma\theta d}{m}\,dt + \frac{\sqrt{2\gamma\theta}}{m}P_i\,dB_i\right]$.

Remedy: add scalar e_n, define evolution such that $H_n + e_n = \mathrm{const}$:

$$dQ_i = \frac{P_i}{m}\,dt, \tag{12a}$$

$$dP_i = -\nabla V(Q_i)\,dt - \sum_{j=1}^{n}\nabla\psi(Q_i-Q_j) - \frac{\gamma}{m}P_i\,dt + \sqrt{2\gamma\theta}\,dB_i, \tag{12b}$$

$$de_n = \frac{1}{n}\sum_{i=1}^{n}\left[\frac{\gamma}{m^2}P_i^2\,dt - \frac{\gamma\theta d}{m}\,dt + \frac{\sqrt{2\gamma\theta}}{m}P_i\,dB_i\right]. \tag{12c}$$

Vlasov-Fokker-Planck equation as GENERIC equation

Macroscopic (PDE) setting

Relevant quantities ($\theta = kT$):

- Hamiltonian $\mathcal{H}(\rho) = \int_{\mathbb{R}^{2d}} \left(\frac{p^2}{2m} + V(q) + \frac{1}{2}(\psi * \rho)(q) \right) \rho \, dqdp$,
- Entropy $\mathcal{S}(\rho) = \theta \int_{\mathbb{R}^{2d}} \rho \log \rho \, dqdp$,

Then consider extended Vlasov-Fokker-Planck equation:

$$\partial_t \rho = -\mathrm{div}_q\Big(\rho \frac{p}{m}\Big) + \mathrm{div}_p \rho \Big(\nabla_q V + \nabla_q \psi * \rho + \gamma \frac{p}{m}\Big) + \gamma\theta\Delta_p \rho, \quad (13)$$

$$\frac{d}{dt} e = \gamma \int_{\mathbb{R}^{2d}} \frac{p^2}{m^2} \rho(dqdp) - \frac{\gamma\theta d}{m}. \quad (14)$$

(Coupling only in one direction: second equation slaved to the first one.)

Vlasov-Fokker-Planck equation as GENERIC equation

GENERIC setting

Proposition

The system (13) *from the previous slide is a GENERIC evolution in* $Z = \mathcal{P}_2(\mathbb{R}^{2d}) \times \mathbb{R}$*, with the following building blocks for* $z = (\rho, e)$*:*

$$\begin{aligned} \mathsf{E}(\rho,e) &= \mathcal{H}(\rho) + e, & \mathsf{L} &= \mathsf{L}(\rho,e) = \begin{pmatrix} \mathsf{L}_{\rho\rho} & 0 \\ 0 & 0 \end{pmatrix}, \\ \mathsf{S}(\rho,e) &= \mathcal{S}(\rho) + e, & \mathsf{K} &= \mathsf{K}(\rho,e) = \gamma \begin{pmatrix} \mathsf{K}_{\rho\rho} & \mathsf{K}_{\rho e} \\ \mathsf{K}_{e\rho} & \mathsf{K}_{ee} \end{pmatrix}, \end{aligned} \tag{15}$$

with (ξ, r) *for* (ρ, e), $\mathsf{L}_{\rho\rho}\xi = \mathrm{div}\rho\mathbf{J}\nabla\xi$ *and*

$$\begin{aligned} \mathsf{K}_{\rho\rho}\xi &= -\mathrm{div}_p \rho \nabla_p \xi, & \mathsf{K}_{\rho e} r &= r\,\mathrm{div}_p\Big(\rho \frac{p}{m}\Big), \\ \mathsf{K}_{e\rho}\xi &= -\int_{\mathbb{R}^{2d}} \frac{p}{m} \cdot \nabla_p \xi \, \rho(dqdp) & \mathsf{K}_{ee} r &= r \int_{\mathbb{R}^{2d}} \frac{p^2}{m^2}\, \rho(dqdp); \end{aligned}$$

$\mathcal{S}(\rho) := -\theta \int_{\mathbb{R}^{2d}} f(x) \log f(x)\, \mathrm{d}x$ *if* ρ *has Lebesgue density* f*;* dE, dS *are* L^2 *gradients.*

(More) general nonequilibrium equations

GENERIC as variational principle

Suggested result (formal for now):
An GENERIC evolution $\{Z, \mathsf{E}, \mathsf{S}, \mathsf{L}, \mathsf{K}\}$,

$$\partial_t z = \mathsf{L}\,\mathrm{d}\mathsf{E} + \mathsf{K}\,\mathrm{d}\mathsf{S}, \tag{16}$$

can be associated with a variational principle. Namely, define

$$2\theta J(z) = \mathsf{S}(z(0)) - \mathsf{S}(z(T)) + \frac{1}{2}\int_0^T \left[\|\partial_t z - \mathsf{L}\,\mathrm{grad}\,\mathsf{E}\|^2_{\mathsf{K}^{-1}} + \|\mathrm{grad}\,\mathsf{S}\|^2_{\mathsf{K}} \right] \mathrm{d}t.$$

Then a function $z\colon [0, T] \to Z$ is a solution of the GENERIC equation (16) iff $J(z) = 0$ (this is a variational principle: next slide!).

Proposition

The formal statement is rigorous for the Vlasov-Fokker-Planck equation.

(All the quantities appearing in the statement are here well-defined.)

Vlasov-Fokker-Planck and GENERIC

Vlasov-Fokker-Planck and large deviations

Proposition

For deterministic initial data $(Q_i(0), P_i(0))$*,* $i = 1, \ldots, n$ *with* $\rho_n(0) \rightharpoonup \rho^0$ *for some* $\rho^0 \in P(\mathbb{R}^{2d})$*, the empirical process* $\{\rho_n\}$ *satisfies a large-deviation principle in the space* $C([0,T], P(\mathbb{R}^{2d}))$*, with good rate function*

$$I(\rho) = \begin{cases} \dfrac{1}{4\gamma\theta} \displaystyle\int_0^T \left\| \partial_t \rho_t - A^{\tau}_{\rho_t} \rho_t \right\|^2_{\rho(t),*} \, \mathrm{d}t & \rho \in AC([0,T]; P(\mathbb{R}^{2d})), \rho|_{t=0} = \rho^0, \\ +\infty & \textit{otherwise}, \end{cases}$$

where $A_\nu f := \frac{p}{m} \cdot \nabla_p f - \left[\nabla_q V + \nabla_q \psi * \nu + \gamma \frac{p}{m} \right] \cdot \nabla_p f + \gamma\theta \Delta_p f.$

Interpretation: Vlasov-Fokker-Planck equation appears as minimiser of rate functional I (this follows from Dawson, Gärtner, *Stochastics*, **20** (1987), 247–308; Budhiraja, Dupuis, Fisher, *Ann. Prob.*, **40** (2012), 74–102)). Up to constant factor, I and J are *identical*.

Vlasov-Fokker-Planck and GENERIC

Summary

- Vlasov-Fokker-Planck equation appears in rate functional for particle process
- One can show (Duong, Peletier, Z.) that this functional can be re-written in GENERIC form, namely for $z = (\rho, e) \in AC([0,T]; Z)$ with $\rho_{t=0} = \rho^0$ as

$$J(z) = \int_0^T \frac{1}{4\theta} \left\| \partial_t z_t - \mathsf{L}(z_t)\,\mathrm{grad}\,\mathsf{E}(z_t) - \mathsf{K}(z_t)\,\mathrm{grad}\,\mathsf{S}(z_t) \right\|^2_{\mathsf{K}(z_t)^{-1}} \mathrm{d}t,$$

  and $J(z) = +\infty$ otherwise.

So in this case the macroscopic GENERIC evolution can be obtained as a large deviation principle (cf. Öttinger, Grmela, *Phys. Rev. E*, **56** (1997), 6633–6655).

Summary

Stochastic first order equation

- Large deviation (saddle point) calculus leads to fluctuating hydrodynamics;

Vlasov-Fokker-Planck and GENERIC

- Large deviation principles can give thermodynamic (GENERIC) evolution;
- scale-bridging reveals variational structure of thermodynamic equation.

Thank you!