Variational methods and up-scaling for GENERIC systems

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Outline

Introduction

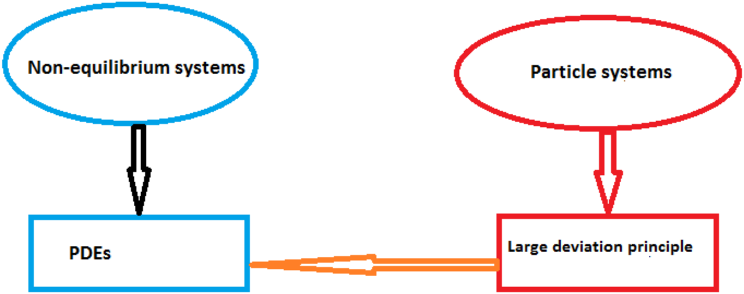
GENERIC

Large deviation principle

Connection between the twos

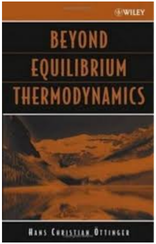
Use of variational structure

Introduction



GENERIC

(General Equation for Non-Equilibrium Reversible-Irreversible Coupling)



GENERIC framework

$$\dot{\mathsf{z}} = \underbrace{\mathsf{L}\,\mathsf{dE}}_{\textit{reversible}} + \underbrace{\mathsf{M}\,\mathsf{dS}}_{\textit{irrevesible}} .$$

- $\mathsf{E}, \mathsf{S} \colon \mathsf{Z} \to \mathbf{R}$ are energy and entropy functionals,
- dE, dS are appropriate derivatives of E and S;
- $\mathsf{L} = -\mathsf{L}^T,\ M = M^T \geq 0$
- $\mathsf{L}\,\mathsf{dS} = 0, \quad \mathsf{M}\,\mathsf{dE} = 0.$

Properties

$$\frac{d\mathsf{E}(\mathsf{z}(t))}{dt} = 0,$$
$$\frac{d\mathsf{S}(\mathsf{z}(t))}{dt} \geq 0.$$

What can we do with GENERIC

- well-accepted framework in physical community.
- very few study from mathematical perspective: Mielke 2011

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(1) Can we derive GENERIC from microscopic particle system?

(2) Existence theory for PDEs using GENERIC structure?

Large deviation principle

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Abel prize 2007

Toss a coin n times:

Large deviation principle

Abel prize 2007

Toss a coin n times:

Probability of observing n heads = $2^{-n} = \exp[-n \log 2]$

$\{X_n\}$ satisfies a large deviation principle with a rate functional I if

$$Prob(X_n \approx x) \approx exp(-nI(x)) \quad \text{as } n \to \infty.$$

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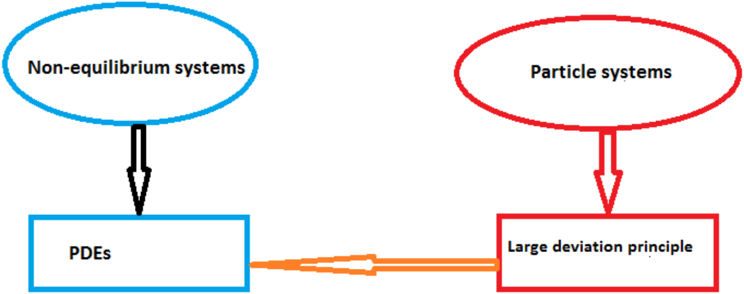
Property of the rate functional:

$$\begin{aligned} &I(x) \geq 0 \quad \forall x, \\ &I(x) = 0 \Rightarrow x \text{ is the most likely event.} \end{aligned}$$


Non-equilibrium systems
Particle systems
PDEs
Large deviation principle

Entropy driven systems.

Diffusion: the Fokker-Planck equation

$$\partial_t \rho = \Delta\rho + \mathrm{div}(\rho\nabla\Psi).$$

JKO1998, Otto2001: Wasserstein gradient flow with respect to the free energy

$$\mathsf{M}d\mathsf{S} := \mathrm{div}(\rho\nabla d\mathsf{S}) := \mathrm{grad}_W d\mathsf{S}(\rho), \quad \mathsf{S}(\rho) = \int (\log\rho + \Psi)\rho,$$

Steepest descent: minimizing the functional

$$K_h(\rho) := \frac{1}{2h} W_2^2(\rho_0, \rho) + S(\rho) - S(\rho_0).$$

Microscopic interpretation of the Wasserstein distance

Many-particle system

$$dX_i(t) = -\nabla\Psi(X_i(t))dt + \sqrt{2}dW_i(t), \quad i = 1, \cdots, n.$$

Empirical measure

$$\rho_n(t) := \frac{1}{n}\sum_{i=1}^{n} \delta_{X_i(t)}.$$

Dawson-Gärtner1987: $\{\rho_n\}$ satisfies a large deviation principle with the rate functional

$$\begin{aligned} I_T(\rho|\rho_0) &= \frac{1}{4}\int_0^T \|\partial_t\rho_t - (\Delta\rho + \mathrm{div}(\rho\nabla\Psi))\|^2_{*,\rho} dt, \\ &= \frac{1}{2}(S(\rho_T) - S(\rho_0)) + \frac{1}{4}\int_0^T (\|\partial_t\rho_t\|^2_{*,\rho} + \|dS\|^2_\rho) dt, \end{aligned}$$

Theorem

$$I_h(\cdot|\rho_0) \approx \frac{1}{2} K_h(\cdot) \quad as \ \ h \to 0,$$

$\approx$: in the sense of Gamma convergence.

AdamDirrPeletierZimmer(Comm. Math. Phys. 2011): for $\Psi \equiv 0$ and for small class of probability measures.

DuongLaschosRenger(ESAIM: COCV. 2013): for quite general Ψ and for much larger class of probability measures.

Energy and entropy driven systems.

The Kramers equation

$$dQ(t) = \frac{P(t)}{m} dt$$

$$dP(t) = \underbrace{-\nabla_q V(Q(t)) dt}_{Potential} \underbrace{-\frac{\gamma}{m} P(t) dt}_{Friction} + \underbrace{\sqrt{2\gamma kT} dW(t)}_{Stochastic\ pertubation}$$

$\rho(t, q, p) =$ the probability of finding the system at position q, momentum p at time t.

$$\partial_t \rho = -\operatorname{div}_q \rho \frac{p}{m} + \operatorname{div}_p \rho \nabla_q V + \gamma \operatorname{div}_p \rho \frac{p}{m} + \gamma k T \Delta_p \rho.$$

Kramers equation in GENERIC framework

Introduce an auxiliary variable e:

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

Reformulation of the extended Kramers equation in GENERIC framework

$$\partial_t \mathsf{z}_t = \mathsf{L}(\mathsf{z}_t)\,\mathrm{grad}\,\mathsf{E}(\mathsf{z}_t) + \mathsf{M}(\mathsf{z}_t)\,\mathrm{grad}\,\mathsf{S}(\mathsf{z}_t),$$

where

$$\mathsf{Z} \;\; = \mathcal{P}_2(\mathbf{R}^{2d}) \times \mathbf{R}, \quad \mathsf{E}(\rho, e) = \mathcal{H}(\rho) + e, \quad \mathsf{L} = \mathsf{L}(\rho, e) = \begin{pmatrix} \mathsf{L}_{\rho\rho} & 0 \\ 0 & 0 \end{pmatrix}$$

$$\mathsf{z} \;\; = (\rho, e), \quad \mathsf{S}(\rho, e) = \mathcal{S}(\rho) + e, \quad \mathsf{M} = \mathsf{M}(\rho, e) = \gamma \begin{pmatrix} \mathsf{M}_{\rho\rho} & \mathsf{M}_{\rho e} \\ \mathsf{M}_{e\rho} & \mathsf{M}_{ee} \end{pmatrix},$$

where the operators defining L and M are given, upon applying them to a vector (ξ, r) at (ρ, e), by

$$\begin{aligned} \mathsf{L}_{\rho\rho}\xi &= \operatorname{div} \rho J \nabla \xi, \quad \mathsf{M}_{\rho\rho}\xi = -\operatorname{div}_p \rho \nabla_p \xi, \quad \mathsf{M}_{\rho e} r = r \operatorname{div}_p \left(\rho \frac{p}{m}\right), \\ \mathsf{M}_{e\rho}\xi &= -\int_{\mathbf{R}^{2d}} \frac{p}{m} \cdot \nabla_p \xi \, \rho(dqdp), \quad \mathsf{M}_{ee} r = r \int_{\mathbf{R}^{2d}} \frac{p^2}{m^2} \, \rho(dqdp). \end{aligned}$$

Particle system

$$dQ_i(t) = \frac{P_i(t)}{m} dt$$
$$dP_i(t) = -\nabla_q V(Q_i(t))dt - \frac{\gamma}{m} P_i(t)dt + \sqrt{2\gamma kT} dW_i(t)$$

Empirical process

$$\rho_n(t, dq, dp) = \frac{1}{n} \sum_{i=1}^{n} \delta_{(Q_i(t), P_i(t))}(dq, dp).$$

Theorem (DuongPeletierZohannesZimmer, Nonlinearity 2013)

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

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

The rate function I can be written in terms of z as

$$I(\mathsf{z}) = \begin{cases} \displaystyle\int_0^T \frac{1}{4\theta} \big\| \partial_t \mathsf{z}_t - \mathsf{L}(\mathsf{z}_t) \operatorname{grad} \mathsf{E}(\mathsf{z}_t) - \mathsf{M}(\mathsf{z}_t) \operatorname{grad} \mathsf{S}(\mathsf{z}_t) \big\|^2_{\mathsf{M}(\mathsf{z}_t)^{-1}} \, dt, \\ \qquad\qquad \text{if } \mathsf{z} = (\rho, e) \in AC([0,T]; \mathsf{Z}) \text{ and } \rho_{t=0} = \rho^0, \\ +\infty \quad \text{otherwise,} \end{cases}$$

in the sense that

$$I\big((\rho, e)\big) = \begin{cases} I(\rho) & \text{provided } t \mapsto \mathcal{H}(\rho_t) + e_t \text{ is constant} \\ +\infty & \text{otherwise.} \end{cases}$$

A variational formulation for GENERIC

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

Variational formulation of a GENERIC system:

Given a GENERIC system $\{\mathsf{Z}, \mathsf{E}, \mathsf{S}, \mathsf{L}, \mathsf{M}\}$*. A function* $\mathsf{z}\colon [0, T] \to \mathsf{Z}$ *is a solution of the GENERIC equation iff* $I(\mathsf{z}) = 0$*.*

How do we use the variational structure to study multi-scale problems?

$$\dot{\mathsf{z}}_\varepsilon = \mathsf{L}_\varepsilon(\mathsf{z}_\varepsilon)\,\mathsf{d}\mathsf{E}_\varepsilon(\mathsf{z}_\varepsilon) + \mathsf{M}_\varepsilon(\mathsf{z}_\varepsilon)\,\mathsf{d}\mathsf{S}_\varepsilon(\mathsf{z}_\varepsilon),$$

Q: $\varepsilon \to 0$?

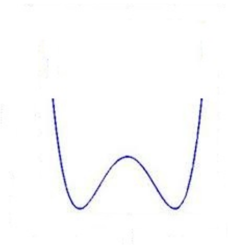
Perturbed Hamiltonian system

$$\partial_t \rho_\epsilon = -\frac{1}{\varepsilon}\,\mathrm{div}_{qp}(\rho_\epsilon J\nabla H) + \Delta_p \rho_\epsilon,$$

where

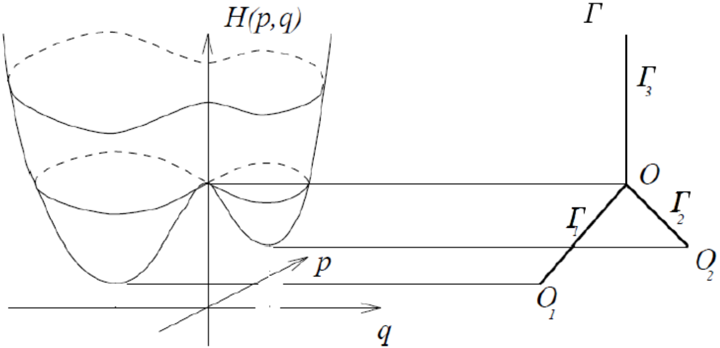
$$q, p \in \mathbb{R},\ H(q,p) = \frac{1}{2}p^2 + V(q).$$

and V is a double-well potential.



Q: What is the behavior of the system when $\varepsilon \to 0$?

Diffusion on graph: Freidlin-Wentzell 1994



Our aim: recover the result of Freidlin-Wentzell using the variational formulation:

$$\rho_\varepsilon \text{ is a solution of the Kramers equation iff } I_\epsilon(\rho_\varepsilon) = 0.$$

By studying Gamma convergence of I_ε, we get the limiting problem.

$$I_\varepsilon(\rho) = \sup_f G_\varepsilon(\rho, f),$$

where

$$G_\varepsilon(\rho, f) = \int_{\mathbb{R}^2} [f_T \rho_T - f_0 \rho_0] - \int_0^T \int_{\mathbb{R}^2} (\partial_t f - \frac{1}{\varepsilon}(J \nabla H) \cdot \nabla f + \Delta_p f + \frac{1}{2} |\nabla_p f|^2) \rho_t \, dt.$$

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Choose $f = g \circ H \Rightarrow J\nabla H \cdot \nabla f = 0$ and we get $G_\varepsilon(\rho, f) \to \hat{G}_0(\hat{\rho}, g)$, with $\hat{\rho} = H_\sharp \rho$ and

$$\hat{G}_0(\hat{\rho}, g) = \int_\Gamma [g_T \hat{\rho}_T - g_0 \hat{\rho}_0] - \int_0^T \int_\Gamma (\partial_t g + A\partial_{hh} g + B\partial_h g + \frac{1}{2}A(\partial_h g)^2)\hat{\rho}_t \, dt.$$

Set $\hat{I}_0(\hat{\rho}) = \sup_g \hat{G}_0(\hat{\rho}, g)$, we obtain the liminf limit

$$\liminf_{\varepsilon \to 0} I_\varepsilon \geq \hat{I}_0.$$

and minimizer of $\hat{I}_0$ is a diffusion on graph Γ:

$$\partial_t \hat{\rho} = \partial_{hh}(A\hat{\rho}) - \partial_h(B\hat{\rho}), \tag{2}$$

for certain A, B computed from H.

Theorem (DuongPeletierSharma 2014: In preparation)

Assume that $\rho_\varepsilon \in C([0,T],P(\mathbb{R}^2))$ *and* $\sup_{\varepsilon>0} I_\varepsilon(\rho_\varepsilon) < \infty$*. Then*

(1) $\hat{\rho}_\varepsilon \rightharpoonup \hat{\rho}_0 \quad$ *in* $C([0,T],P(\Gamma))$*,*

(2) $\hat{\rho}_0$ *solves* (2) *.*

Summary and Future work

Summary

1. Connection between physical structure of PDEs with particle models via large deviation principle
2. Suggested a variational formulation for GENERIC and its application
3. The method obtains both the limiting equation and the fluctuation simultaneously.

Future work

Apply the method for other (nonlinear) systems (ODEs, PDEs, SDEs)

Answer question 2) at the beginning.

Thank you for your attention