

From simple particle models to PDE dynamics

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GENERIC

General nonequilibrium equations

Nonequilibrium framework (GENERIC)

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

$$\partial_t z = L(z) dE(z) + K(z) dS(z), \quad (1)$$

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

$$\{\{F_1, F_2\}_L, F_3\}_L + \{\{F_2, F_3\}_L, F_1\}_L + \{\{F_3, F_1\}_L, F_2\}_L = 0$$

for all functions $F_i: Z \rightarrow \mathbb{R}$, with Poisson bracket $\{\cdot, \cdot\}_L$

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

- ▶ $K = K(z)$ is symmetric and positive semidefinite.

General nonequilibrium equations

Nonequilibrium framework (GENERIC)

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

$$L dS = 0, \quad K dE = 0. \quad (2)$$

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

$$\begin{aligned} \frac{dE(z(t))}{dt} &= dE \cdot \frac{dz}{dt} = dE \cdot (L dE + K dS) = 0, \\ \frac{dS(z(t))}{dt} &= dS \cdot \frac{dz}{dt} = dS \cdot (L dE + K dS) = dS \cdot K dS \geq 0. \end{aligned}$$

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

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, ...).

Example of a GENERIC system

Thermoviscoelasticity

$$u_{tt} = ku_{xx} + \alpha\theta_x + \mu u_{xxt} - \gamma u_{xxxx}$$

$$\theta_t = \kappa\theta_{xx} + \alpha\theta u_{xt} + \mu u_{xt}^2$$

(+ initial and boundary conditions). Then with $p = \dot{u}$

$$E = \int_{\Omega} \left[\frac{1}{2} p^2 + \theta + \frac{k}{2} u_x^2 + \frac{\gamma}{2} u_{xx}^2 \right] dx,$$

$$S = \int_{\Omega} [\log \theta - \alpha u_x] dx$$

Mielke, *Contin. Mech. Thermodyn.*, **23** (2011), 233–256: write

$L = Q_S L_0 Q_S^*$, $K = Q_E K_0 Q_E^*$, with given k_{visc} and k_{heat} ,

$$L_0 = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad K_0 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & k_{\text{visc}} & 0 \\ 0 & 0 & k_{\text{heat}} \end{pmatrix}.$$

Example of a GENERIC system

Thermoviscoelasticity

$$Q_S = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -\frac{1}{D_\theta S} D_u S[\cdot] & -\frac{1}{D_\theta S} D_p S[\cdot] & \frac{1}{D_\theta S} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -\theta D_u S[\cdot] & 0 & \theta \end{pmatrix},$$

which yields

$$\begin{aligned} Q_S^* dE &= \begin{pmatrix} 1 & 0 & -\theta \star \partial_u S \\ 0 & 1 & 0 \\ 0 & 0 & \theta \end{pmatrix} \begin{pmatrix} \partial_u E \\ \partial_p E \\ \partial_\theta E \end{pmatrix} \\ &= \begin{pmatrix} k u_{xx} - \gamma u_{xxxx} - \theta \star \partial_u S \\ p \\ \theta \end{pmatrix} = \begin{pmatrix} k u_{xx} - \gamma u_{xxxx} - \alpha \theta u_x \\ p \\ \theta \end{pmatrix}, \end{aligned}$$

which is the *driving force*.

Purely entropic systems

Particles and deterministic gradient flows

From particles to diffusion

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

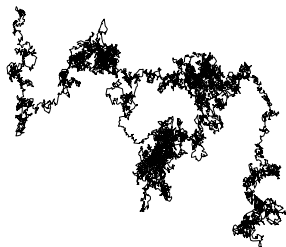


Figure: Brownian motion,
taken from Mörters & Peres,
Brownian Motion

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 with diffusion constant κ ,

$$\begin{aligned}\frac{\partial}{\partial t}\rho(x, t) &= \kappa\Delta\rho(x, t) \\ &= \kappa\operatorname{div}\left(\rho(x, t)\nabla\frac{\delta S}{\delta\rho}(\rho)\right)\end{aligned}\tag{3}$$

with **entropy**

$$S(\rho) := \int_{\mathbb{R}^n} \rho(x) \log \rho(x) \, dx.$$

Question: How can we *derive (3) and stochastic “corrections” directly from particles?*

Diffusion as entropic gradient flow

Jordan, Kinderlehrer & Otto, 1998

$$\Delta\rho = \operatorname{div} \left(\rho \nabla \frac{\delta S}{\delta \rho} \right) = -\operatorname{grad}_W S(\rho) = -\textit{Wasserstein gradient of } S.$$

Variational formulation: for linear diffusion

$$\frac{\partial}{\partial t} \rho(x, t) = \Delta \rho(x, t), \quad (4)$$

via time-stepping, define at time k the function ρ^k as minimiser of

$$K_h(\rho; \rho^{k-1}) := \frac{1}{2h} d(\rho, \rho^{k-1})^2 + S(\rho),$$

where d is the *Wasserstein metric*

$$d(\rho_0, \rho_1)^2 := \inf_{\gamma \mid \pi_0 \gamma = \rho_0, \pi_1 \gamma = \rho_1} \int_{\mathbb{R}^n \times \mathbb{R}^n} (x - y)^2 \gamma(dx dy).$$

This approximation converges to the solution ρ of (4) as $h \rightarrow 0$.

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*

$$\text{Prob}(\rho_n \approx \rho) \sim \exp[-nJ(\rho)], \quad \text{as } n \rightarrow \infty, \quad (5)$$

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

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

Is there a 'dynamic Sanov' (away from equilibrium, time step $h > 0$)?

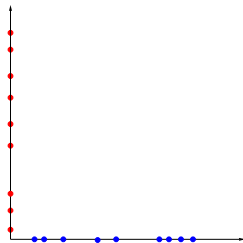
Dynamics: The microscopic picture

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

$$p_h(x, y) := \frac{1}{2\sqrt{\pi h}} e^{-(y-x)^2/4h}.$$

Possible particle jumps:



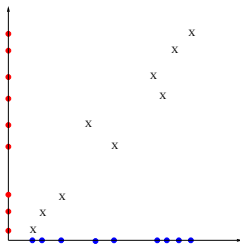
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Possible particle jumps:



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

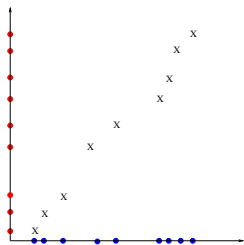
Dynamics: The microscopic picture

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

$$p_h(x, y) := \frac{1}{2\sqrt{\pi h}} e^{-(y-x)^2/4h}.$$

Possible particle jumps:



Jumps maximise

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

$$\inf_{\gamma \in \Gamma(\rho_0, \rho_1)} \int_{\mathbb{R}^n \times \mathbb{R}^n} (x - y)^2 \gamma(dx dy),$$

$$\Gamma(\rho_0, \rho) = \{ \gamma \in \mathcal{M}_1(\mathbb{R}^n \times \mathbb{R}^n) : \\ \pi_0 \gamma = \rho_0, \pi_1 \gamma = \rho \}.$$

Dynamics: From particles to the gradient flow

Large deviation principle

Let $L_n^t = n^{-1} \sum_{i=1}^n \delta_{X^{(i)}(t)}$ be the empirical measure of n Brownian particles.

Let $L_n^0 \approx \rho_0$ and consider the *large deviation principle* describing the probability to approximate at time h a measure ρ by L_n^h :

$$\mathbb{P}(L_n^h \approx \rho \mid L_n^0 \approx \rho_0) \approx \exp[-nJ_h(\rho; \rho_0)] \quad \text{as } n \rightarrow \infty.$$

Here the *rate function* J_h is (Léonard; Adams, Peletier, Dirr & Z.)

$$J_h(\rho; \rho_0) := \inf_{q: \pi_0 q = \rho_0, \pi_1 q = \rho} H(q \mid q_0)$$

with

$$H(q \mid p) := \begin{cases} \int_{\mathbb{R} \times \mathbb{R}} f(x, y) \log f(x, y) p(d(x, y)) & \text{if } q \ll p, f = \frac{dq}{dp} \\ +\infty & \text{else} \end{cases}.$$

What has the rate functional J_h to do with the time discretisation

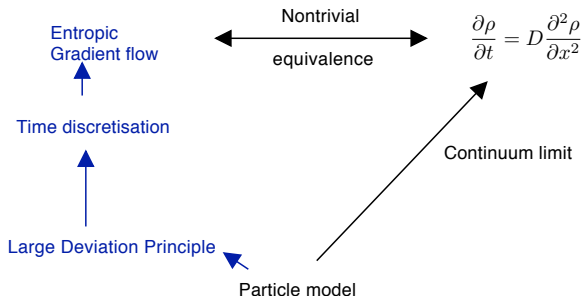
$K_h(\rho; \rho^{k-1}) := \frac{1}{2h} d(\rho, \rho^{k-1})^2 + S(\rho)$ of Otto's entropic flow?

Dynamics: From particles to the gradient flow

What has the rate functional J_h to do with the time discretisation K_h of Otto's entropic flow?

Theorem (Adams, Dirr, Peletier, Z. / Dirr, Laschos, Z.)

J_h and K_h agree asymptotically in the limit $h \rightarrow 0$, in the sense of Γ -convergence [ADPZ: Measures on a flat torus with Lebesgue density in $\{\rho \in L^\infty(0, L) : \int_0^L \rho dx = 1 \text{ and } \|\rho - L^{-1}\|_\infty < \delta\}$, for suitable $0 < \delta < 1$; DLZ: Gaussian measures].



Large deviations: from particles to PDEs

Dawson-Gärtner theorem

Now let us consider the *dynamic* situation:

Given n Brownian particles and a fixed terminal time $T > 0$, consider the path of *empirical measures* $[0, T] \ni t \mapsto \rho_n(t) = \frac{1}{n} \sum_{j=1}^n \delta_{X(t,j)}$.

Then (Dawson, Gärtner, *Mem. Amer. Math. Soc.*, **78** (1989); Kipnis, Olla, *Stochastics Rep.*, **33** (1990), 17–25):

$$\text{Prob}(\rho_n \approx \rho) \sim \exp[-nJ(\rho)], \quad (6)$$

with the *rate functional*

$$J(\rho) := \frac{1}{2} \int_0^T \left\| \frac{\partial \rho}{\partial t} - \Delta \rho \right\|_{\rho(t),*}^2 dt \quad (7)$$

(the norm will be defined later).

- ▶ Limit particle number $n \rightarrow \infty$: (6) gives vanishing probability to all states ρ except those for which $J(\rho) = 0$, the solution of the heat equation.

Pathwise approach

Large deviation principle for paths

Re-write the functional from the previous slide by expanding the square:

$$\begin{aligned} & \frac{1}{2} \int_0^T \left\| \frac{\partial \rho}{\partial t} - \Delta \rho \right\|_{\rho, *}^2 dt \\ &= \frac{1}{2} \int_0^T \left[\left\| \frac{\partial \rho}{\partial t} \right\|_{\rho, *}^2 - 2 \left(\frac{\partial \rho}{\partial t}, \Delta \rho \right)_{\rho, *} + \|\Delta \rho\|_{\rho, *}^2 \right] dt \\ &= S(\rho(T)) - S(\rho(0)) + \frac{1}{2} \int_0^T \left[\left\| \frac{\partial \rho}{\partial t} \right\|_{\rho, *}^2 + \|\Delta \rho\|_{\rho, *}^2 \right] dt \\ &= S(\rho(T)) - S(\rho(0)) + \frac{1}{2} \int_0^T \left[\left\| \frac{\partial \rho}{\partial t} \right\|_{\rho, *}^2 + \left\| -\frac{\delta S}{\delta \rho} \right\|_{\rho}^2 \right] dt; \end{aligned}$$

here we used

$$\Delta \rho = \operatorname{div} \rho \nabla \left(\frac{\delta S}{\delta \rho} \right) = -\operatorname{grad}_W S(\rho) = -\text{Wasserstein gradient of } S.$$

Insight: *the mixed term gives the entropy* (but we need to recognise it).

Nonlinear diffusion, boundary conditions: preprint by Bodineau, Lebowitz, Mouhot and Villani.

Simplest energy- and entropy-driven system

(More) general nonequilibrium equations

Vlasov-Fokker-Planck equation

Duong, Peletier, Z.: Revisit Vlasov-Fokker-Planck equation in light of GENERIC equation (1), $\rho = \rho(p, q)$.

$$\partial_t \rho = -\operatorname{div}_q \left(\rho \frac{p}{m} \right) + \operatorname{div}_p \rho \left(\nabla_q V + \nabla_q \psi * \rho + \gamma \frac{p}{m} \right) + \gamma \theta \Delta_p \rho. \quad (8)$$

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

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

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

Vlasov-Fokker-Planck equation as GENERIC equation

Microscopic energy balance

The VFP equation (8) 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 $dH_n = -\frac{1}{n} \sum_{i=1}^n \left[\frac{\gamma}{m^2} P_i^2 dt - \frac{\gamma\theta d}{m} dt + \frac{\sqrt{2\gamma\theta}}{m} P_i dW_i \right]$.

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

$$dQ_i = \frac{P_i}{m} dt, \quad (9a)$$

$$dP_i = -\nabla V(Q_i) dt - \sum_{j=1}^n \nabla \psi(Q_i - Q_j) - \frac{\gamma}{m} P_i dt + \sqrt{2\gamma\theta} dW_i, \quad (9b)$$

$$de_n = \frac{1}{n} \sum_{i=1}^n \left[\frac{\gamma}{m^2} P_i^2 dt - \frac{\gamma\theta d}{m} dt + \frac{\sqrt{2\gamma\theta}}{m} P_i dW_i \right]. \quad (9c)$$

Vlasov-Fokker-Planck equation as GENERIC equation

GENERIC setting

Proposition

The system (9) 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 $z = (\rho, e)$:

$$\begin{aligned} E(\rho, e) &= \mathcal{H}(\rho) + e, & L &= L(\rho, e) = \begin{pmatrix} L_{\rho\rho} & 0 \\ 0 & 0 \end{pmatrix}, \\ S(\rho, e) &= \mathcal{S}(\rho) + e, & K &= K(\rho, e) = \gamma \begin{pmatrix} K_{\rho\rho} & K_{\rho e} \\ K_{e\rho} & K_{ee} \end{pmatrix}, \end{aligned} \quad (10)$$

with (ξ, r) for (ρ, e) , $L_{\rho\rho}\xi = \operatorname{div} \rho \mathbf{J} \nabla \xi$ and

$$\begin{aligned} K_{\rho\rho}\xi &= -\operatorname{div} \rho \nabla \rho \xi, & K_{\rho e} r &= r \operatorname{div} \rho \left(\rho \frac{p}{m} \right), \\ K_{e\rho}\xi &= -\int_{\mathbb{R}^{2d}} \frac{p}{m} \cdot \nabla \rho \xi \rho(dqdp) & K_{ee} r &= r \int_{\mathbb{R}^{2d}} \frac{p^2}{m^2} \rho(dqdp); \end{aligned}$$

$\mathcal{S}(\rho) := -\theta \int_{\mathbb{R}^{2d}} f(x) \log f(x) dx$ 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 $\{Z, E, S, L, K\}$,

$$\partial_t z = L dE + K dS, \quad (11)$$

can be associated with a variational principle. Namely, define

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

Then a function $z: [0, T] \rightarrow Z$ is a solution of the GENERIC equation (11) iff $J(z) = 0$.

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 $(Q_i(0), P_i(0))$, $i = 1, \dots, n$ 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

$$I(\rho) = \begin{cases} \frac{1}{4\gamma\theta} \int_0^T \|\partial_t \rho_t - A_{\rho_t}^T \rho_t\|_{-1, \rho_t}^2 dt & \rho \in AC([0, T]; P(\mathbb{R}^{2d})), \rho|_{t=0} = \rho^0, \\ +\infty & \text{otherwise,} \end{cases}$$

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

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

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).

Noise

Extracting more information

The key argument revisited

We consider two objects:

- ▶ Continuum description (e.g., K_h , variational time-discrete formulation of PDE),
- ▶ Rate functional J_h .

The theorem said: these are *asymptotically* equivalent (in the sense of Γ -convergence); but $J_h \neq K_h$!

In time-continuous setting:

$$J(\rho) := \frac{1}{2} \int_0^T \left\| \frac{\partial \rho}{\partial t} - \frac{\partial^2 \rho}{\partial x^2} \right\|_{\rho, *}^2 dt$$

Rate functionals J and J_h describes fluctuations and contains *more* information than the PDE.

Question: how can we use this additional information?

Extracting more information: Noise

Rate functional contains “more” information than time-step from PDE. How to extract this information? Preliminary answer (with Rob Jack, Physics, Bath, v. Renesse): stochastic equation.

Dean's equation (Dean, *J. Phys. A: Math. Gen.*, **29** (1996), L613–L617)

$$\frac{\partial \rho}{\partial t} = \Delta \rho + \frac{1}{n} \operatorname{div}(\sqrt{\rho} \dot{W}) \quad (12)$$

with space-time white noise \dot{W} . Saddle point argument: (12) gives for $n \rightarrow \infty$ the Wasserstein formulation of the diffusion equation (time discretisation, limiting action functional has integrand $\left\| \frac{\partial \rho}{\partial t} - \Delta \rho \right\|_{\rho, *}^2$).

In other words:

1. The noise $\operatorname{div}(\sqrt{\rho} \dot{W})$ is the “right” noise from the perspective of the Wasserstein geometry (Sturm, von Renesse, *Ann. Probab.*, **37** (2009), 1114–1191)
2. It can formally be derived by a large deviation principle.

Open questions:

1. Other noises (e.g., from different particle model with the same hydrodynamic limit)
2. Procedure applicable for other equations?

References

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Thank you!