Scaling limits of stochastic dynamics of particle systems in continuum

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Based on a joint paper with Y. Kondratiev and O. Kutoviy
and on a joint paper with D. Finkelshtein and Y. Kondratiev

Continuous particle system

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We denote by Γ the set of all possible configurations γ.
Γ is called configuration space.

Kawasaki dynamics

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describes the rate at which the particle x of the configuration γ hops to y.

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describes the rate at which the particle x of the configuration γ hops to y.

The generator of the corresponding Markov process is given by

$$(LF)(\gamma) = \sum_{x \in \gamma} \int_{\mathbb{R}^d} c(x, y, \gamma)\big(F(\gamma \setminus x \cup y) - F(\gamma)\big)\, dy.$$

Equilibrium Markov processes

$X = (X_t)_{t \geq 0}$ a Markov process on Γ.

X is equilibrium:
Assume that the initial distribution of a particle system is μ (which is a probability measure on Γ).
Then at each moment of time $t > 0$, X_t has the same distribution μ, i.e., the distribution of the system at each moment of time does not change.
μ is called invariant measure for the process X.

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We will be interested in the case where μ is a Gibbs measure on Γ.

Gibbs measures

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The interaction between particles is described through a potential of pair interaction:

$$\phi : \mathbb{R}^d \setminus \{0\} \to \mathbb{R}, \qquad \phi(-x) = \phi(x).$$

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If $\{x_n\}_{n=1}^N$ is a finite system of particles, then the interaction energy is equal to

$$E\left(\{x_n\}_{n=1}^N\right) = \sum_{1 \le i < j < \le N} \phi(x_i - x_j).$$

Relative energy of interaction

For an infinite system of particles $\gamma = \{x_n\}_{n=1}^{\infty}$, the interaction energy is informally given by

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Relative energy of interaction between a particle y and a configuration $\gamma = \{x_n\}_{n=1}^{\infty}$:

$$E(y \mid \gamma) = \sum_{n=1}^{\infty} \phi(x_n - y).$$

Poisson measure

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For any bounded set $\Delta \subset \mathbb{R}^d$ and $\gamma \in \Gamma$, define

$$X_\Delta(\gamma) = |\gamma \cap \Delta| \quad \text{(the number of points of } \gamma \text{ in } \Delta).$$

Poisson measure

Poisson measure π_z is a probability measure on Γ which is uniquely characterized through the following properties:

- For each bounded $\Delta \subset \mathbb{R}^d$, the random variable X_Δ has Poisson distribution with parameter $z\,\mathrm{vol}(\Delta)$, i.e.,

$$\pi_z(X_\Delta = k) = \exp[-z\,\mathrm{vol}(\Delta)]\,\frac{(z\,\mathrm{vol}(\Delta))^k}{k!}$$

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- For any bounded, mutually disjoint sets

  $$\Delta_1, \ldots, \Delta_m \subset \mathbb{R}^d,$$

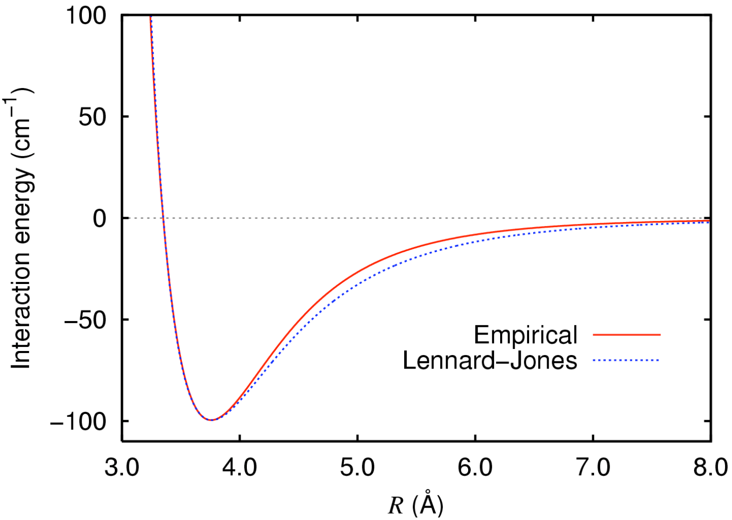
  the random variables $X_{\Delta_1}, \ldots, X_{\Delta_m}$ are independent under μ_z:

  $$\begin{aligned}\pi_z(&X_{\Delta_1} = k_1,\, X_{\Delta_2} = k_2 \ldots, X_{\Delta_m} = k_m)\\ &= \pi_z(X_{\Delta_1} = k_1)\pi_z(X_{\Delta_2} = k_2)\cdots\pi_z(X_{\Delta_m} = k_m).\end{aligned}$$

Gibbs measure

Interaction between particles, $\phi \not\equiv 0$.
Typical example: Lennard–Jones potential

$$\phi(x) = c\left[\left(\frac{\sigma}{|x|}\right)^{12} - \left(\frac{\sigma}{|x|}\right)^{6}\right].$$


100
50
0
−50
−100
Interaction energy (cm−1)
3.0
4.0
5.0
6.0
7.0
8.0
R (Å)
Empirical
Lennard–Jones

Gibbs measure

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$$\mu(d\gamma) = \frac{1}{Z} \exp[-E(\gamma)]\, \pi_z(d\gamma).$$

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A possible rigorous definition: Georgii–Nguyen–Zessin identity:

$$\int_\Gamma \mu(d\gamma) F(\gamma) \sum_{x\in\gamma} \psi(x) = \int_\Gamma \mu(d\gamma) \int_{\mathbb{R}^d} z\, dx \exp\left[-E(x \mid \gamma)\right] F(\gamma \cup x)\psi(x)$$

for arbitrary functions $F : \Gamma \to [0, \infty)$ and $\psi : \mathbb{R}^d \to [0, +\infty)$.

Balance condition

Recall

$$(LF)(\gamma) = \sum_{x \in \gamma} \int_{\mathbb{R}^d} c(x, y, \gamma)\big(F(\gamma \setminus x \cup y) - F(\gamma)\big)\, dy.$$

Balance condition

Recall

$$(LF)(\gamma) = \sum_{x\in\gamma} \int_{\mathbb{R}^d} c(x,y,\gamma)\big(F(\gamma \setminus x \cup y) - F(\gamma)\big)\, dy.$$

For the corresponding dynamics to have a Gibbs measure μ as invariant measure the following balance condition should be satisfied for any $x, y \in \mathbb{R}^d$ and $\gamma \in \Gamma$:

$$c(x,y,\gamma\cup x)\exp[-E(x \mid \gamma)] = c(y,x,\gamma\cup y)\exp[-E(y \mid \gamma)]$$

Kawasaki dynamics

We fix a parameter $s \in [0, 1]$.
Our choice:

$$c(x, y, \gamma) = a(x - y) \exp[\,(1 - s)E(x \mid \gamma \setminus x) - sE(y \mid \gamma \setminus x)\,]$$

Here, the function $a : \mathbb{R}^d \to [0, \infty)$ satisfies

$$a(x) = \tilde{a}(|x|)$$

and

$$a(x) = 0 \quad \text{if } |x| > 1.$$

Free Kawasaki dynamics

Special case $\phi \equiv 0$:

$$c(x, y, \gamma) = c(x, y) = a(x - y)$$

This is a dynamics of independent hopping particles in $\mathbb{R}^d$, where the jump rate from x to y is equal to $a(x - y)$.

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In the case $\phi \not\equiv 0$, the particles interact and the jump rate of each individual particle depends on the rest of the configuration.

Diffusive scaling limit

We start with Kawasaki dynamics

$$X = \big(X(t)\big)_{t\geq 0}$$

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$$a_\varepsilon(x) := \frac{1}{\varepsilon^d} \, a\left(\frac{x}{\varepsilon}\right)$$

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Resulting dynamics

$$X_\varepsilon = \big(X_\varepsilon(t)\big)_{t \geq 0}$$

Diffusive scaling limit

Next we re-scale time:

$$Y_\varepsilon(t) = X_\varepsilon\left(\frac{t}{\varepsilon^2}\right)$$

If ε is small, the Y_ε dynamics is 'quicker' than the X_ε dynamics.

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The jump rate corresponding to the Y_ε dynamics:

$$c_\varepsilon(x, y, \gamma) = \frac{1}{\varepsilon^{d+2}}\, a\left(\frac{x-y}{\varepsilon}\right) \exp\left[\,(1-s)E(x \mid \gamma\backslash x) - sE(y \mid \gamma\backslash x)\,\right]$$

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We denote by L_ε the corresponding generator:

$$(L_\varepsilon F)(\gamma) = \sum_{x\in\gamma} \int_{\mathbb{R}^d} c_\varepsilon(x,y,\gamma)\big(F(\gamma\setminus x\cup y) - F(\gamma)\big)\, dy.$$

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Limiting diffusion has generator

$$\begin{aligned}
&L^{\mathrm{dif}} F(\{x_n\}_{n=1}^{\infty}) \\
&= \sum_{n=1}^{\infty} \Bigg(\frac{1}{2} \Delta_n F(\{x_n\}_{n=1}^{\infty}) - s \sum_{m \neq n} \langle \nabla_m F(\{x_n\}_{n=1}^{\infty}), \nabla \phi(x_n - x_m) \rangle \Bigg) \\
&\qquad \times \exp\left[(-2s+1) \sum_{i \neq n} \phi(x_n - x_i) \right].
\end{aligned}$$

In fact, we have for each $F \in \mathcal{F}$

$$\int_{\Gamma} \left(L_\varepsilon F(\gamma) - L^{\mathrm{dif}} F(\gamma)\right)^2 \mu(d\gamma) \to 0 \quad \text{as } \varepsilon \to 0.$$

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If there exists a unique Markov process on Γ whose generator on $\mathcal{F}$ is equal to L^{dif}, then the finite-dimensional distributions of the scaled process Y_ε converge to the finite-dimensional distributions of the diffusion process X^{dif} with generator L^{dif}. This means that, for any moments of time

$$0 \le t_1 < t_2 < \cdots < t_n$$

the joint distribution of

$$Y_\varepsilon(t_1),\ Y_\varepsilon(t_2), \dots,\ Y_\varepsilon(t_n)$$

is 'close' for small ε to the joint distribution of

$$X^{\mathrm{dif}}(t_1), X^{\mathrm{dif}}(t_2), \dots, X^{\mathrm{dif}}(t_n)$$

Case $s = \frac{1}{2}$: gradient stochastic dynamics

Limiting generator:

$$L^{\mathrm{dif}} F(\{x_n\}_{n=1}^{\infty}) = \sum_{n=1}^{\infty} \left(\frac{1}{2} \Delta_n F(\{x_n\}_{n=1}^{\infty}) - \frac{1}{2} \sum_{m \neq n} \langle \nabla_m F(\{x_n\}_{n=1}^{\infty}), \nabla \phi(x_n - x_m) \rangle \right)$$

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This dynamics informally solves the following infinite system of SDEs:

$$dx_i(t) = dB_i(t) - \frac{1}{2} \sum_{j \neq i} \nabla \phi(x_i(t) - x_j(t)),$$

$$x_i(0) = x_i, \quad i \in \mathbb{N},$$

$$\{x_i\}_{i=1}^{\infty} \in \Gamma \text{ is } \mu\text{-distributed}$$

where $B_i(t)$, $i \in \mathbb{N}$, are independent standard Brownian motions on $\mathbb{R}^d$.

Free Brownian particles

If $\phi = 0$, we have

$$dx_i(t) = dB_i(t), \quad i \in \mathbb{N}$$

so that we have a dynamics of independent Brownian particles.

Deterministic gradient dynamics of n particles

Dynamics of n charged particles interacting through potential ϕ:

$$dx_i(t) = -\frac{1}{2} \sum_{i \neq j} \nabla \phi\big(x_i(t) - x_j(t)\big)\, dt,$$

$$x_i(0) = x_i \qquad i = 1, \ldots, n,$$

Stochastic gradient dynamics of n particles

Dynamics of n charged particles interacting through potential ϕ suspended in water:

$$dx_i(t) = dB_i(t) - \frac{1}{2}\sum_{i \neq j} \nabla \phi(x_i(t) - x_j(t))\, dt,$$
$$x_i(0) = x_i \qquad i = 1, \ldots, n,$$

The terms $dB_i(t)$ describe the influence of ‘small’ molecules of water on the ‘big’ charged particles.

Case $s = 0$

Limiting generator:

$$L^{\mathrm{dif}} F(\{x_n\}_{n=1}^{\infty}) = \sum_{n=1}^{\infty} \frac{1}{2} \Delta_n F(\{x_n\}_{n=1}^{\infty}) \exp\left[\sum_{m \neq n} \phi(x_n - x_m)\right]$$

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$$dx_i(t) = \exp\left[\frac{1}{2} \sum_{j \neq i} \phi(x_i(t) - x_j(t))\right] dB_i(t), \quad i \in \mathbb{N}.$$

(no drift term, interaction is in the diffusion coefficient)

BAD scaling of Kawasaki dynamics

Again we start with Kawasaki with

$$c(x, y, \gamma) = a(x - y) \exp\left[(1 - s)E(x, \gamma \setminus x) - sE(y, \gamma \setminus x)\right],$$

where $s \in [0, 1]$.

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where $s \in [0, 1]$.

We scale the function a:

$$a_\varepsilon = \varepsilon^d a(\varepsilon x)$$

Note that

$$a_\varepsilon(x) = 0 \quad \text{if } |x| > \frac{1}{\varepsilon}$$

and

$$\int_{\mathbb{R}^d} a_\varepsilon(x)\, dx = \int_{\mathbb{R}^d} a(x)\, dx.$$

We do not scale time!

Resulting dynamics

$$X_\varepsilon = \big(X_\varepsilon(t) \big)_{t \geq 0}$$

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The jump rate corresponding to the X_ε dynamics:

$$c_\varepsilon(x, y, \gamma) = \varepsilon^d \, a\,(\varepsilon(x - y)) \exp\left[\,(1-s)E(x \mid \gamma \setminus x) - sE(y \mid \gamma \setminus x)\,\right]$$

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$$(L_\varepsilon F)(\gamma) = \sum_{x\in\gamma} \int_{\mathbb{R}^d} c_\varepsilon(x, y, \gamma)\big(F(\gamma\setminus x \cup y) - F(\gamma)\big)\, dy.$$

BAD scaling of Kawasaki dynamics

We are interested in the limit as $\varepsilon \to 0$.
Normalization condition:

$$\int_{\mathbb{R}^d} a(x)\, dx = 1$$

Glauber dynamics

The limiting dynamics: Glauber dynamics (spatial birth-and-death process)

$$(L^G F)(\gamma) = C_s \Bigg(\sum_{x\in\gamma} d(x,\gamma)(F(\gamma\setminus x) - F(\gamma)) + \int_{\mathbb{R}^d} z\, dy\, b(y,\gamma)(F(\gamma\cup y) - F(\gamma)) \Bigg),$$

where

$$d(x,\gamma) = \exp\big[sE(x,\gamma\setminus x)\big],$$
$$b(y,\gamma) = \exp\big[-(1-s)E(y,\gamma)\big]$$

and

$$C_s := \int_\Gamma \exp\left[-(1-s)\sum_{x\in\gamma}\phi(x)\right]\mu(d\gamma)$$

Case $s = 0$

Then

$$C_0 := \int_\Gamma \mu(d\gamma) \exp\left[-\sum_{x\in\gamma} \phi(x) \right] = k^{(1)},$$

(the first correlation function of the Gibbs measure μ) and

$$(L^G F)(\gamma) = k^{(1)} \Bigg(\sum_{x\in\gamma} (F(\gamma\setminus x) - F(\gamma)) + \int_{\mathbb{R}^d} z\, dy\, \exp\big[-E(y,\gamma) \big] (F(\gamma\cup y) - F(\gamma)) \Bigg)$$

Free Glauber dynamics

Let $\phi \equiv 0$. Then $\mu = \pi_z$ (Poisson measure), $k^{(1)} = z$,

$$(L^G F)(\gamma) = k^{(1)} \Bigg(\sum_{x \in \gamma} (F(\gamma \setminus x) - F(\gamma)) + \int_{\mathbb{R}^d} z \, dy \, (F(\gamma \cup y) - F(\gamma)) \Bigg)$$

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Additionally new particle are randomly born, so that the Poisson point process over $\mathbb{R}^d \times (0, \infty)$ with intensity measure $z\,dx\,dt$ describes positions in $\mathbb{R}^d$ and times in $(0, \infty)$ where and when new particles are born.

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Each new particle y, born at time $\tau > 0$, randomly dies, so that the probability that the particle y is still alive at time $\tau + t$ is e^{-t}.

Diffusive scaling vs. BAD scaling

Diffusive scaling is 'point-wise':
When we start Kawasaki dynamics at a fixed configuration γ the scaled dynamics will converge to the diffusive dynamics starting at γ.

E.g.: in the free Kawasaki dynamics, dynamics of each separate particle converges to a Brownian motion.

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BAD scaling is not 'point-wise':
It only holds for equilibrium dynamics whose initial distribution is a Gibbs measure μ.

E.g.: in the free Kawasaki dynamics, the dynamics of each separate particle under the BAD scaling converges to a random death process: the particle either does not hop (stays alive) or hops to infinity (dies). No new particle is born.