Discrete solid-on-solid models

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Discrete processes, stochastic PDEs, deterministic PDEs

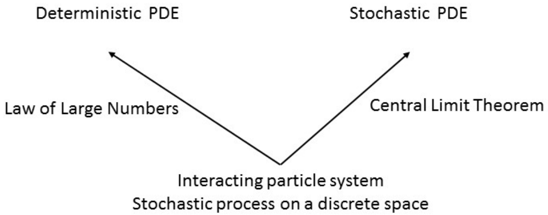
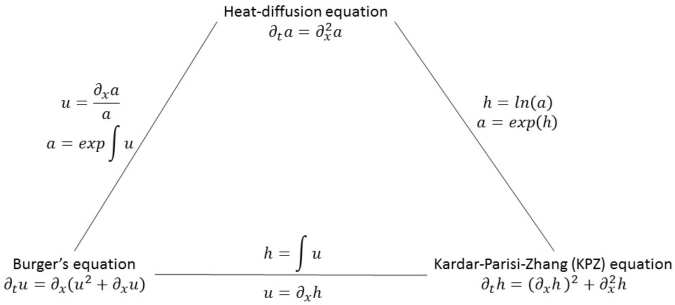


Table: Deterministic PDEs

Heat-diffusion equation $\partial_t a = \partial_x^2 a$	Linear 4th order diffusion equ $\partial_t a = -\partial_x^4 a$
Burger's equation $\partial_t u = \partial_x(u^2 + \partial_x u)$	Chan-Hilliard equation $\partial_t u = \partial_x^2(f(u) - \partial_x^2 u)$
Karder-Parisi-Zhang (KPZ) equation $\partial_t h = (\partial_x h)^2 + \partial_x^2 h$	4th order KPZ equation $\partial_t h = \partial_x(f(\partial_x h) - \partial_x^3 h)$

Second order PDEs



Fourth order PDEs

4th order diffusion equation

$$\partial_t a = -\partial_x^4 a$$

Cahn-Hilliard equation
for phase transition in a binary alloy

$$\partial_t u = \partial_x^2 (f(u) - \partial_x^2 u)$$

$$f(u) = u^3 - u$$

$$h = \int u$$

$$u = \partial_x h$$

4th order KPZ equation

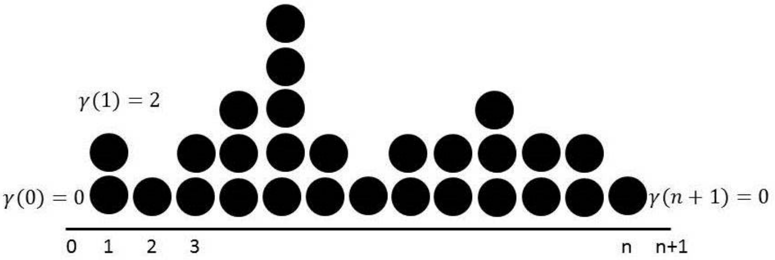
$$\partial_t h = \partial_x (f(\partial_x h) - \partial_x^3 h)$$

Deterministic eq	Stochastic eq	Discrete process
Heat-diffusion	Stochastic heat Brownian motion	Random walk
Burger's	Stochastic Burger's	WAS EP
KPZ	Stochastic KPZ wavelets	WASS SOSP
4th order KPZ	4th order stochastic KPZ	FTNP SOSP

Discrete Solid-on-Solid model with fixed total number of particle: **Configuration**

Particle configuration: $\gamma = (\gamma(0), \gamma(1), \ldots, \gamma(n))$ with $\gamma(i)$ being the number of particles at position i.

Total number of particles is fixed: $\gamma(0) + \gamma(1) + \cdots + \gamma(n) = K$



Discrete Solid-on-Solid model with fixed total number of particle: **Energy**

Energy of a configuration:

$$E(\gamma) = \sum_{i=1}^{n+1} V\big(\gamma(i-1) - \gamma(i)\big)$$

with some positive function V, like $|x|$ or x^2.

Flat interfaces have low energy and rough interfaces have high energy.

Discrete Solid-on-Solid model with fixed total number of particle: **Partition function**

Relative frequency of a particle configuration γ when the system is at equilibrium:

$$\mu(\gamma) = \frac{1}{Z_\beta} \exp\left\{ -\beta \sum_{i=1}^{n+1} V\big(\gamma(i-1) - \gamma(i)\big) \right\}$$

with partition function Z_β, a normalizing factor to ensure that relative frequencies of all configurations add up to 1.

Knowledge of the partition function is necessary for many interesting physical quantities (like average energy of the system)

Discrete solid-on-solid model with fixed total number of particle: **Kawasaki dynamics**

Use Metropolis-Hasting algorithm and Gibbs sampler to construct an irreducible, aperiodic Markov chain or process that converges to the distribution $\mu(\gamma)$. The process makes moves according to

- Kawasaki dynamics: randomly select two sites *i* and *j* and replace the particles at these sites by *k* and *l* particles where $k + l = \gamma(i) + \gamma(j)$

$$(\gamma(i), \gamma(j)) \to (k, l)$$

Gibbs sampler: Move only to neighboring configurations. Use conditional distributions of configuration distribution $\mu(\gamma)$ as transition probabilities.

Mixing time of a Markov process

For a reversible Markov process on Ω_n with stationary distribution μ we measure the convergence rate via

$$\tau(\epsilon) = \min\{t : \|\nu_t^\gamma - \mu\| \leq \epsilon, \ \ \forall \gamma \in \Omega_n\}$$

where ν_t^γ is the distribution of the configuration at time t starting from configuration γ at time 0, and $\|\cdot\|$ denotes variation distance. The process convergence rate is measured by the time until the variation distance from μ drops to ϵ, for an arbitrary configuration.

Coupling

- Two distribution:
  Let μ and ν be two distributions. A coupling of μ and ν is a specification of a joint distribution with μ and ν as its marginal distributions.
- Two copies of the same Markov process:
  Coupling is defined by running two copies of the same Markov process such that each copy has the marginals as those of the given Markov process

Coupling Lemma

If there exists a monotone coupling $(X_t, Y_t)_{t \geq 0}$ such that for some time t_0 and for every two configurations γ_1 and γ_2,

$$P(X_{t_0} \neq Y_{t_0} | X_0 = \gamma_1, Y_0 = \gamma_2) \leq \epsilon$$

then the mixing time $\tau(\epsilon) \leq t_0$.

Monotone coupling of Kawasaki dynamics

can be achieved in 3 steps:

- identify a **partial order**, $\preccurlyeq$, on configuration space, hyperplane $\Omega_{n,K}$
- construct **functions** $f : \Omega_{n,K} \to \Omega_{n,K}$ on configuration space that preserve partial order

$$\gamma \preccurlyeq \xi \Longrightarrow f(\gamma) \preccurlyeq f(\xi)$$

- find a **random mechanism** to select such functions in agreement with Kawasaki dynamics transition probabilities

Partial order

Example 1

$$\gamma \preccurlyeq_1 \xi \Longleftrightarrow \gamma_0 \geq \xi_0 \quad \gamma_1 \leq \xi_1 \quad \cdots \quad \gamma_n \leq \xi_n$$

Example 2

$$\gamma \preccurlyeq_2 \xi \Longleftrightarrow \gamma_1 - \gamma_0 \geq \xi_1 - \xi_0 \quad \gamma_2 - \gamma_1 \leq \xi_2 - \xi_1 \quad \cdots$$

$$\cdots \quad \gamma_n - \gamma_{n-1} \leq \xi_n - \xi_{n-1}$$

Both partial orders on the hyperplane have a minimal element $(K, 0, \ldots, 0)$ and NO maximal element

Coupling of Kawasaki dynamics

Function

For a fixed bond $i \longleftrightarrow i+1$ and number $U \in [0,1]$ define f

$$\begin{array}{c}(\gamma_0, \dots, \gamma_{i-1}, \gamma_i, \gamma_{i+1}, \gamma_{i+2} \dots, \gamma_n) \\ f \downarrow \\ (\gamma_1, \dots, \gamma_{i-1}, x, y, \gamma_{i+2}, \dots, \gamma_n)\end{array}$$

Identification of x and y

- $x + y = \gamma_i + \gamma_{i+1} = T$
- x is largest integer such that cumulative distribution of $p(\gamma_i, \gamma_{i+1}) = \mu(\gamma_i, \gamma_{i+1} \mid \gamma_0, \dots, \gamma_{i-1}, \gamma_{i+2} \dots, \gamma_n)$ satisfies

$$p(0,T) + p(1,T) + \cdots + p(x-1, y+1) + p(x,y) \leq U$$

Random mechanism

Bond $i \longleftrightarrow i+1$ is uniformly selected from all possible near neighbor bonds $1 \longleftrightarrow 2$, $2 \longleftrightarrow 3$, $\ldots$, $n-1 \longleftrightarrow n$, $n \longleftrightarrow 0$.
U is uniformly selected from $[0,1]$.

Issues regarding the coupling of Kawasaki dynamics

- Is this coupling monotone? Are the functions used to couple the Kawasaki dynamics order-preserving? Is there any stochastic domination between the two-site conditional probabilities of the equilibrium probability?
- Can the partial order on the hyperplane be modified so that it has a minimal and maximal element and the coupling is monotone?
- If a monotone coupling cannot be identified can the non-monotone coupling be used to calculate the mixing time of the Markov process?

Work in progress: discrete SOS with Kawasaki dynamics

- study the properties of the proposed coupling
- if possible, identify "the most efficient" coupling, a coupling that minimizes the probability that the two copies differ from each other
- estimate the mixing time
- estimate the spectral gap