Online probability seminar, Seoul (Online)

Metastable dynamics of one-dimensional Allen–Cahn-type equations

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INSTITUT ORLÉANS · TOURS Mathématiques & Physique Théorique DENIS POISSON

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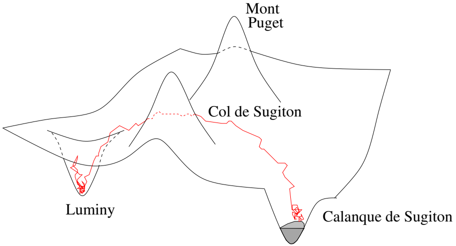
Joint works with Bastien Fernandez (Paris) and Barbara Gentz (Bielefeld)

Project PERIS-TOCH

1. Reversible SDEs:

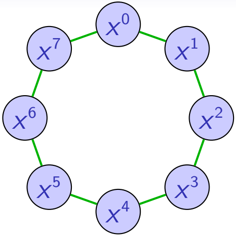
The potential-theoretic approach to metastability



A particle system

[B, Fernandez, Gentz, Nonlinearity 2007]

- N particles on a circle $\mathbb{Z}/N\mathbb{Z}$
- Bistable local dynamics
- Ferromagnetic nearest neighbour coupling
- Independent noise on each site



$$\mathrm{d}x_t^i = \left[x_t^i - (x_t^i)^3\right]\mathrm{d}t + \frac{\gamma}{2}\left[x_t^{i+1} - 2x_t^i + x_t^{i-1}\right]\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t^i$$

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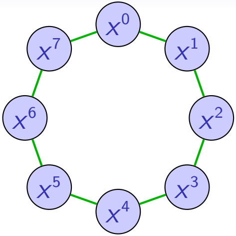

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Gradient system $\qquad \mathrm{d}x_t = -\nabla V(x_t)\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t$

potential $V(x) = \sum_i U(x^i) + \frac{\gamma}{4}\sum_i (x^{i+1} - x^i)^2 \qquad U(\xi) = \frac{1}{4}\xi^4 - \frac{1}{2}\xi^2$

Coarsening dynamics with noise

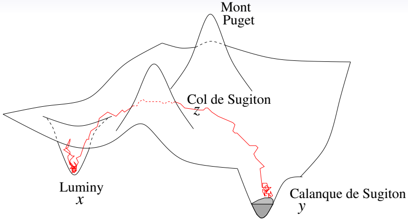
(Link to simulation)

Reversible diffusion in a double-well

$$\mathrm{d}x_t = -\nabla V(x_t)\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t$$

$V : \mathbb{R}^d \to \mathbb{R}$ confining potential

$\tau_y^x = \inf\{t > 0 \colon x_t \in \mathcal{B}_\varepsilon(y)\}$
first-hitting time of small ball $\mathcal{B}_\varepsilon(y)$, when starting in x



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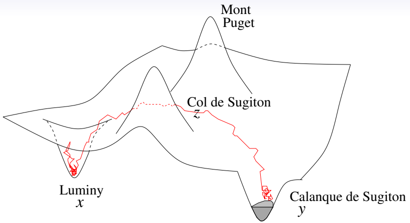

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Arrhenius' law (1889): $\mathbb{E}[\tau_y^x] \simeq \mathrm{e}^{[V(z)-V(x)]/\varepsilon}$

Eyring–Kramers law (1935, 1940):
Eigenvalues of Hessian of V at minimum x: $0 < \nu_1 \leqslant \nu_2 \leqslant \dots \leqslant \nu_d$
Eigenvalues of Hessian of V at saddle z: $\lambda_1 < 0 < \lambda_2 \leqslant \dots \leqslant \lambda_d$

$$\mathbb{E}[\tau_y^x] = 2\pi\sqrt{\frac{\lambda_2 \dots \lambda_d}{|\lambda_1|\nu_1 \dots \nu_d}}\,\mathrm{e}^{[V(z)-V(x)]/\varepsilon}\big[1 + \mathcal{O}_\varepsilon(1)\big]$$

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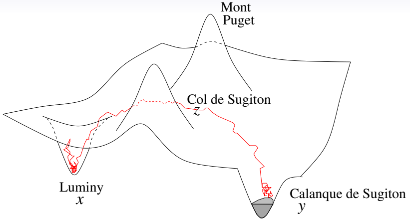

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Arrhenius' law: proved by [Freidlin, Wentzell, 1979] using large deviations

Eyring–Kramers law: [Bovier, Eckhoff, Gayrard, Klein, 2004] using potential theory, [Helffer, Klein, Nier, 2004] using Witten Laplacian, ...

Potential-theoretic proof

$$\mathrm{d}x_t = -\nabla V(x_t)\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t$$

- Generator: $\mathcal{L} = \varepsilon\Delta - \nabla V \cdot \nabla = \varepsilon\,\mathrm{e}^{V/\varepsilon}\,\nabla \cdot \mathrm{e}^{-V/\varepsilon}\,\nabla$
- Invariant probability: $\pi(\mathrm{d}x) = \frac{1}{Z}\,\mathrm{e}^{-V(x)/\varepsilon}\,\mathrm{d}x \quad \Rightarrow \quad \mathcal{L}^\dagger\pi = 0$

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- Reversible: $\langle f, \mathcal{L}g\rangle = \langle \mathcal{L}f, g\rangle$ for $\langle f, g\rangle = \int_{\mathbb{R}^d} \mathrm{e}^{-V(x)/\varepsilon} f(x)g(x)\,\mathrm{d}x$
- Dirichlet form: $\mathcal{E}(f) = \langle f, -\mathcal{L}f\rangle = \varepsilon\int_{\mathbb{R}^d} \mathrm{e}^{-V(x)/\varepsilon}|\nabla f(x)|^2\,\mathrm{d}x$
  $\mathcal{E}(f,g) = \langle f, -\mathcal{L}g\rangle$

Expected hitting time

- Expected hitting time:

$$w_A(x) = \mathbb{E}^x[\tau_A] \quad \text{satisfies} \quad \begin{cases} (\mathcal{L}w_A)(x) = -1 & x \in A^c \\ w_A(x) = 0 & x \in A \end{cases}$$

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- Green function:

$$\begin{cases} (\mathcal{L}G_A)(x) = \delta(x-y) & x \in A^c \\ G_A(x,y) = 0 & x \in A \end{cases}$$

$$\Rightarrow \qquad w_A(x) = -\int_{A^c} G_A(x,y)(\mathrm{d}y)$$

Committor

- ▷ Committor:

$$h_{AB}(x) = \mathbb{P}^x\{\tau_A < \tau_B\} \quad \text{satisfies} \quad \begin{cases} (\mathcal{L}h_{AB})(x) = 0 & x \in (A \cup B)^c \\ h_{AB}(x) = 1 & x \in A \\ h_{AB}(x) = 0 & x \in B \end{cases}$$

- ▷ Equilibrium measure: $e_{AB}(\mathrm{d}x) = (-\mathcal{L}h_{AB})(\mathrm{d}x)$ measure on $x \in \partial A$

$$\Rightarrow \qquad h_{AB}(x) = -\int_A G_B(x,y) e_{AB}(\mathrm{d}y)$$

Capacity

Capacity: $\mathrm{cap}(A, B) = \int_{\partial A} \mathrm{e}^{-V(x)/\varepsilon}\, e_{AB}(\mathrm{d}x)$

$\Rightarrow \nu_{AB}(\mathrm{d}x) = \frac{1}{\mathrm{cap}(A,B)}\, \mathrm{e}^{-V(x)/\varepsilon}\, e_{AB}(\mathrm{d}x)$ is a probability measure on ∂A

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Theorem ("Magic" formula):

$$\mathbb{E}^{\nu_{AB}}[\tau_B] := \int_{\partial A} \mathbb{E}^x[\tau_B] \nu_{AB}(\mathrm{d}x) = \frac{1}{\mathrm{cap}(A,B)} \int_{B^c} \mathrm{e}^{-V(x)/\varepsilon} \, h_{AB}(x) \, \mathrm{d}x$$

Dirichlet principle

Theorem: Dirichlet principle

Let $\mathcal{H}_{AB} = \{h : \mathbb{R}^d \to [0,1] : h|_A = 1, h|_B = 0\}$. Then

$$\operatorname{cap}(A, B) = \inf_{h \in \mathcal{H}_{AB}} \mathcal{E}(h) = \mathcal{E}(h_{AB})$$

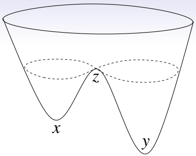
Thomson principle

Theorem: Thomson principle [Landim, Mariani, Seo 2018]

Let $\mathcal{U}_{AB} = \{f \colon \nabla \cdot f|_{(A\cup B)^c} = 0, \int_{\partial A} f(x) \cdot n_A(x) \sigma(\mathrm{d}x) = 1\}$. Then

$$\mathrm{cap}(A,B) = \sup_{f \in \mathcal{U}_{AB}} \frac{1}{\mathcal{D}(f)} = \frac{1}{\mathcal{D}(f_{AB})} \qquad \mathcal{D}(f) = \frac{1}{\varepsilon} \int \mathrm{e}^{V(x)/\varepsilon} |f(x)|^2 \,\mathrm{d}x$$

Proof of Eyring–Kramers law



$$\mathrm{d}x_t = -\nabla V(x_t)\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t$$

▷ A, B small balls around x, y

Potential landscape for the particle system

$$V(x) = \sum_{i \in \mathbb{Z}/N\mathbb{Z}} U(x^i) + \frac{\gamma}{4} \sum_{i \in \mathbb{Z}/N\mathbb{Z}} (x^{i+1} - x^i)^2 \qquad U(\xi) = \tfrac{1}{4}\xi^4 - \tfrac{1}{2}\xi^2$$

$\gamma = 0$: $\mathcal{X} = \{-1, 0, 1\}^N$, $\mathcal{X}_0 = \{-1, 1\}^N$, $\mathcal{X}_1 = \{x \in \mathcal{X} : \text{one } x^i = 0\}$

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Theorem [BFG, Nonlinearity 2007]

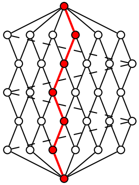
No bifurcation for $0 \leqslant \gamma \leqslant \gamma^*(N)$

where $\gamma^*(N) > \frac14 \quad \forall N \geqslant 2$

$V_\gamma(z^*_\gamma) = V_0(z^*_0) + \gamma(\#$ interfaces$) + \cdots$

Ising-like dynamics

+	+	+	+	+	+
−	+	+	+	+	+
−	+	+	+	+	−
−	+	+	+	−	−
−	−	+	+	−	−
−	−	+	−	−	−
−	−	−	−	−	−



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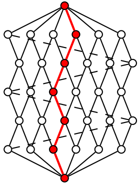
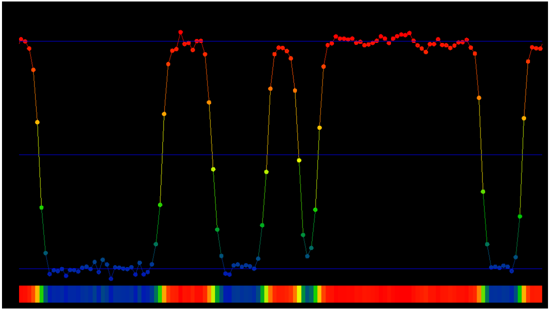


Theorem [BFG, Nonlinearity 2007]

$\gamma > \dfrac{1}{2\sin^2(\pi/N)} \Leftrightarrow \mathcal{X}_0 = \{\pm(1, \dots, 1)\}$, $\mathcal{X}_1 = \{0\} \Leftrightarrow$ Synchronization

2. The stochastic Allen–Cahn PDE on the 1d torus



Deterministic Allen–Cahn PDE

[Chafee & Infante 74, Allen & Cahn 75]

$$\partial_t u(t,x) = \Delta u(t,x) + f(u(t,x))$$

- $x \in [0, L]$, L: bifurcation parameter
- $u(t,x) \in \mathbb{R}$
- Either periodic or zero-flux Neumann boundary conditions
- In this talk: $f(u) = u - u^3$ (results more general)

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Energy function:

$$V[u] = \int_0^L \Big[\frac{1}{2}u'(x)^2 - \frac{1}{2}u(x)^2 + \frac{1}{4}u(x)^4\Big]\,\mathrm{d}x \qquad \to \ \text{min}$$

Scaling limit of particle system with $\gamma = 2\frac{N^2}{L^2}$

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Scaling limit of particle system with $\gamma = 2\frac{N^2}{L^2}$

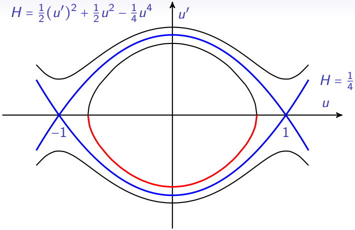
Stationary solutions: $u_0''(x) = -u_0(x) + u_0(x)^3$ critical points of V

Stability: Sturm–Liouville problem $\partial_t v_t(x) = v_t''(x) + [1 - 3u_0(x)^2]v_t(x)$

Stationary solutions

$u_0''(x) = -f(u_0(x)) = -u_0(x) + u_0(x)^3$

- $u_\pm(x) \equiv \pm 1$
- $u_0(x) \equiv 0$
- Nonconstant solutions satisfying b.c. (expressible in terms of Jacobi elliptic fcts)



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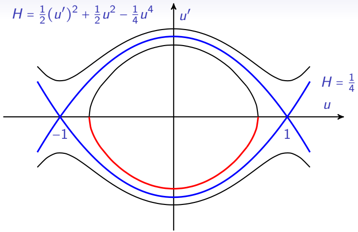
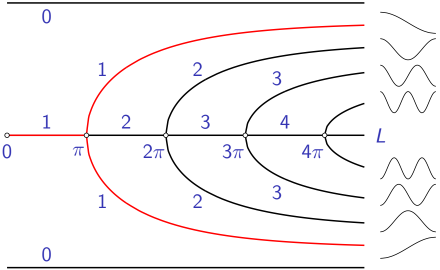


- ▷ Neumann b.c: $2k$ nonconstant solutions when $L > k\pi$

Number of positive eigenvalues
(= unstable directions)
Transition state



- ▷ Periodic b.c: k families when $L > 2k\pi$

Eyring–Kramers law for 1D SPDEs: heuristics

$$\partial_t u(t,x) = \Delta u(t,x) + f(u(t,x)) \quad + \sqrt{2\varepsilon}\,\xi(t,x) \qquad (f(u) = u - u^3)$$

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Initial condition: u_{in} near $u_- \equiv -1$ with eigenvalues $\nu_k = (\frac{\beta k \pi}{L})^2 + 2$

Target: $u_+ \equiv 1$, $\tau_+ = \inf\{t > 0 \colon \|u_t - u_+\|_{L^\infty} < \rho\}$

Transition state: ($\beta = 1$ for Neumann b.c., $\beta = 2$ for periodic b.c.)

$$u_{\text{ts}}(x) = \begin{cases} u_0(x) \equiv 0 & \text{if } L \leqslant \beta\pi \quad \text{with ev } \lambda_k = (\frac{\beta k\pi}{L})^2 - 1 \\ u_1(x) \ \beta\text{-kink stationary sol.} & \text{if } L > \beta\pi \quad \text{with ev } \lambda_k' \end{cases}$$

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[Faris & Jona-Lasinio 82]: large-deviation principle

$\Rightarrow$ Arrhenius law: $\mathbb{E}^{u_{\rm in}}[\tau_+] \simeq \mathrm{e}^{(V[u_{\rm ts}] - V[u_-])/\varepsilon}$

[Maier & Stein 01]: formal computation; for Neumann b.c.

$$\Rightarrow \mathbb{E}^{u_{\rm in}}[\tau_+] \simeq 2\pi \sqrt{\frac{1}{|\lambda_0|\nu_0} \prod_{k=1}^{\infty} \frac{\lambda_k}{\nu_k}}\, \mathrm{e}^{(V[u_{\rm ts}] - V[u_-])/\varepsilon}$$

Eyring–Kramers law for 1D SPDEs: heuristics

Eyring–Kramers law for 1D SPDEs: main result

Theorem: Neumann b.c. [B & Gentz, 2013]

- If $L < \pi - c$ with $c > 0$, then

$$\mathbb{E}^{u_{\text{in}}}[\tau_+] = 2\pi \sqrt{\frac{1}{|\lambda_0|\nu_0} \prod_{k=1}^{\infty} \frac{\lambda_k}{\nu_k}} \, \mathrm{e}^{(V[u_{\text{ts}}]-V[u_-])/\varepsilon} \Big[1 + \underbrace{\mathcal{O}(\varepsilon^{1/2}|\log\varepsilon|^{3/2})}_{\text{error not optimal}}\Big]$$

- If $L > \pi + c$, then same formula with extra factor $\frac{1}{2}$ (since 2 saddles) and λ'_k instead of λ_k

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- If $L > \pi + c$, then same formula with extra factor $\frac{1}{2}$ (since 2 saddles) and λ_k' instead of λ_k

- Results also for L near π and periodic b.c.
- Prefactor involves a Fredholm determinant:
  $\Delta_\perp$ Laplacian acting on mean zero functions

$$\prod_{k=1}^{\infty}\frac{\lambda_k}{\nu_k} = \det\bigl[(-\Delta_\perp - 1)(-\Delta_\perp + 2)^{-1}\bigr] = \det\bigl[\mathbb{1} - 3(-\Delta_\perp + 2)^{-1}\bigr]$$

  converges because $\log\det = \operatorname{Tr}\log$ and $(-\Delta_\perp + 2)^{-1}$ is trace class (limit $= \frac{\sqrt{2}\sin(L)}{\sinh(\sqrt{2}L)}$)

Ideas of the proof ($L < \pi$)

▷ Spectral Galerkin approximation: $u(t,x) = \sum_{|k| \leqslant N} z_k(t) e_k(x)$ (Fourier)

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- Spectral Galerkin approximation: $u(t,x) = \sum_{|k|\leqslant N} z_k(t) e_k(x)$ (Fourier)
- Change of variables $u(x) = u_0 + \sqrt{\varepsilon} u_\perp(x)$ where $\int_0^L u_\perp(x)\,\mathrm{d}x = 0$

$$\Rightarrow \frac{1}{\varepsilon} V[u_0 + \sqrt{\varepsilon} u_\perp] = \frac{1}{\varepsilon} \underbrace{\left(\frac{1}{4} u_0^4 - \frac{1}{2} u_0^2\right)}_{V_0(u_0)} + Q_{u_0}[u_\perp] + \sqrt{\varepsilon} R_{u_0}[u_\perp]$$

where

$$\begin{cases} Q_{u_0}[u_\perp] = \dfrac{1}{2} \displaystyle\int_0^L \left[u_\perp'(x)^2 - (1 - 3u_0^2) u_\perp(x)^2\right] \mathrm{d}x = \dfrac{1}{2} \langle u_\perp, [-\Delta - (1 - 3u_0^2)] u_\perp \rangle \\ R_{u_0}[u_\perp] = u_0 \displaystyle\int_0^L u_\perp(x)^3 \,\mathrm{d}x + \sqrt{\varepsilon} \int_0^L u_\perp(x)^4 \,\mathrm{d}x \qquad \text{(remainder)} \end{cases}$$

Ideas of the proof ($L < \pi$)

- ▷ Spectral Galerkin approximation: $u(t,x) = \sum_{|k| \leqslant N} z_k(t) e_k(x)$ (Fourier)
- ▷ Change of variables $u(x) = u_0 + \sqrt{\varepsilon} u_\perp(x)$ where $\int_0^L u_\perp(x) \, \mathrm{d}x = 0$

$$\Rightarrow \frac{1}{\varepsilon} V[u_0 + \sqrt{\varepsilon} u_\perp] = \frac{1}{\varepsilon} \underbrace{\left(\frac{1}{4} u_0^4 - \frac{1}{2} u_0^2 \right)}_{V_0(u_0)} + Q_{u_0}[u_\perp] + \sqrt{\varepsilon} R_{u_0}[u_\perp]$$

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- ▷ Dirichlet principle with $h = h(u_0)$ s.t. $h'(u_0) = -\frac{1}{c} \mathrm{e}^{V_0(u_0)/\varepsilon}$, $c \simeq \sqrt{\frac{2\pi\varepsilon}{|\lambda_0|}}$

$$\operatorname{cap}(A, B) \leqslant \mathcal{E}(h) = \frac{\varepsilon^{1 + \frac{N}{2}}}{c^2} \int_{-1}^{1} \mathrm{e}^{V_0(u_0)/\varepsilon} \underbrace{\int \mathrm{e}^{-Q_{u_0}[u_\perp]} \, \mathrm{e}^{-\sqrt{\varepsilon} R_{u_0}[u_\perp]} \, \mathrm{d}u_\perp}_{= \sqrt{\frac{(2\pi)^N}{\det[-\Delta_\perp - (1 - 3u_0^2)]}} \mathbb{E}^{\gamma}[\mathrm{e}^{-\sqrt{\varepsilon} R_{u_0}}]} \, \mathrm{d}u_0$$

Ideas of the proof ($L < \pi$)

- Thomson principle with divergence-free unit flow $f = K^{-1}\,\mathrm{e}^{-Q_0[u_\perp]}\,e_{u_0}$

  Normalisation $K = \varepsilon^{\frac{N}{2}} \displaystyle\int \mathrm{e}^{-Q_0[u_\perp]}\,\mathrm{d}u_\perp = \sqrt{\frac{(2\pi\varepsilon)^N}{\det[-\Delta_\perp - 1]}}$

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- Conclusion: $\operatorname{cap}(A,B) = \varepsilon \sqrt{\frac{|\lambda_0|}{2\pi\varepsilon}} \sqrt{\frac{(2\pi\varepsilon)^N}{\det[-\Delta_\perp - 1]}} \bigl[1 + \mathcal{O}(\varepsilon)\bigr]$

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Other elements of the proof:

- A priori bounds on h_{AB}: large deviations (or symmetry argument)
- Convergence of hitting times as $N \to \infty$: a priori estimate for $\mathbb{E}[\tau_B^2]$
- Coupling argument for start in u_{in} [Martinelli, Olivieri & Scoppola]
- Bifurcation at $L = \beta\pi$

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Thanks for your attention!

Slides available at `https://www.idpoisson.fr/berglund/Seoul23a.pdf`