MJP $X_t \in \Omega$ embedded in $\mathbb{R}^d$ (e.g. $\mathbb{Z}^d$)

R reaction channels with

- rates $\lambda_j(x)$
- change vectors ν_j $\quad j = 1..R.$

$x \in S \Rightarrow x + \nu_j \in \Omega$

Dynamics:

$$X_{t+\Delta t} \mid X_t = \begin{cases} X_t + \nu_j & \text{with prob } \Delta t\, \lambda_j(X_t) + o(\Delta t) \\ & j = 1..R \\ X_t & \text{with prob } 1 - \Delta t \sum_{j=1}^{R} \lambda_j(X_t) + o(\Delta t) \end{cases}$$

Generator:

$$(L\phi)(x) = \lim_{t \downarrow 0} \frac{1}{t} \mathbb{E}^x[\phi(X_t) - \phi(x)]$$

$$= \sum_{j=1}^{R} \lambda_j(x) [\phi(x + \nu_j) - \phi(x)] \quad .$$

Since:

$$\mathbb{E}^x \phi(X_t) = \sum_{j=1}^{R} t\lambda_j(x) \phi(x + \nu_j) + \left(1 - \sum_{j=1}^{R} t\lambda_j(x)\right) \phi(x) + o(t)$$

Simulations: rejection free KMC:

Gillespie / BKL.

$$X_t \to X_{t+\tau(X_t)} = X_t + \nu_{j(X_t)} \to \dots$$

$$\begin{cases} \tau(X_t) = \text{exp. with rate } \lambda_0(X_t) = \sum_{j=1}^{R} \lambda_j(X_t) \\ j(X_t) = \text{drawn from } p_j(X_t) = \dfrac{\lambda_j(X_t)}{\sum_{k=1}^{R} \lambda_k(X_t)} \end{cases}$$

NB. More generally. $X_t \in \mathbb{R}^d$. $z \in \mathbb{R}^p$

$$(L\phi)(x) = \frac{1}{\varepsilon}\int \lambda(x,z)\,[\phi(x+\varepsilon\nu(z)) - \phi(x)]\,\mu(dz)$$

some prob. meas.

ex: 1. Schlögl model

$$A + S \underset{k_3}{\overset{k_2}{\rightleftharpoons}} 3S$$

$$S \underset{k_0}{\overset{k_1}{\rightleftharpoons}} B$$

N = # mol of species S

$\frac{N}{V}$ = concentration

C_A, C_B = concentration of A, B.

$N \to N+1$
$$\begin{cases} k_0 V C_B & \nu = +1. \\ k_2 C_A \frac{N(N-1)}{V} & \nu = +1 \end{cases}$$

$N \to N-1$
$$\begin{cases} k_3 \frac{N(N-1)(N-2)}{V^2} & \nu = -1 \\ k_1 N & \nu = -1 \end{cases}$$

scaling: $N \gg 1$, $V \gg 1$, $\frac{N}{V} = x = O(1)$

$\Rightarrow$ $\varepsilon = 1/V \ll 1$ &

$$\begin{cases} \lambda_+^\varepsilon(x) = k_0 + k_1 x(x-\varepsilon) & \nu_+ = +1 \\ \lambda_-^\varepsilon(x) = k_1 x + k_3 x(x-\varepsilon)(x-2\varepsilon) & \nu_- = -1 \end{cases}$$

2. discrete diffusion:

N_T particles in M boxes.

N_i = # particle in box $i = 1 .. M$. $\left(\sum_{i=1}^{M} N_i = N_T\right)$

jump right $N_i \to N_i - 1$ & $N_{i+1} \to N_{i+1} + 1$ rate αN_i

jump left $N_i \to N_i - 1$ & $N_{i-1} \to N_{i-1} + 1$ rate αN_i

α = cst.

$$\boxed{\begin{array}{l} \partial_i^R = \begin{array}{c} \begin{pmatrix} 0 & .. & -1 & +1 & .. & 0 \end{pmatrix} \\ \quad\quad\quad\; i \quad\;\; i+1 \end{array} \\ \partial_i^L = \begin{array}{c} \begin{pmatrix} 0 & .. & +1 & -1 & .. & 0 \end{pmatrix} \\ \quad\quad\quad\; i-1 \quad\; i \end{array} \end{array}}$$

periodic.

$N = 1/\varepsilon$

scaling: $N_T \gg 1$ $N_i \gg 1$ $\frac{N_i}{N} = x_i = O(1)$

$\Rightarrow$ $\varepsilon = 1/N \ll 1$ &

$$\boxed{(\mathcal{L} f)(x) = \frac{\alpha}{\varepsilon} \sum_{i=1}^{M} \left(x^i \left[f(x + \varepsilon \partial_i^R) - f(x) \right] + x^i \left[f(x + \varepsilon \partial_i^L) - f(x) \right] \right)}$$

Rescaled generator

$$(L^{\varepsilon}\phi)(x) = \sum_{j=1}^{R} \frac{1}{\varepsilon}\lambda_j^{\varepsilon}(x)\,[\phi(x+\varepsilon\nu_j) - \phi(x)].$$

with: $\lambda_j^{\varepsilon}(x) = \lambda_j(x) + \varepsilon\tilde{\lambda}_j(x) + O(\varepsilon^2).$

BKE $\mathbb{E}^{x} F(X_t^{\varepsilon}) = u^{\varepsilon}(T-t, x).$

$$\partial_t u^{\varepsilon} + L^{\varepsilon} u^{\varepsilon} = 0 \qquad u^{\varepsilon}(T,x) = F(x)$$

$$\|$$

$$\partial_t u^{\varepsilon}(t,x) + \frac{1}{\varepsilon}\sum_{j=1}^{R} \lambda_j^{\varepsilon}(x)\,[u^{\varepsilon}(t, x+\varepsilon\nu_j) - u^{\varepsilon}(t,x)] = 0$$

NB forward KE : $p(t,x)$ = PROB that $X_t = x$ @ time t

$$\partial_t p(t,x) = \sum_{j=1}^{R} [\lambda_j(x-\nu_j)\,p(t, x-\nu_j) - \lambda_j(x)\,p(t,x)]$$

LLN

$$u^\varepsilon \xrightarrow[\varepsilon \downarrow 0]{} u$$

$$\boxed{\partial_t u(t,x) + \sum_{j=1}^{R} \lambda_j(x)\, \nu_j \cdot \nabla u(t,x) = 0}$$

Since: $\frac{1}{\varepsilon}\left[u(t, x+\varepsilon \nu_j) - u(t,x)\right] = \nu_j \cdot \nabla u(t,x) + O(\varepsilon)$

BKE for ODE:

$$\boxed{\dot{X}_t = \sum_{j=1}^{R} \lambda_j(X_t)\, \nu_j}$$

Law of mass action

CLT ... linear SDE with coeff dep. on X_t, $\lambda(x)$ & $\tilde{\lambda}(x)$

LDP

$$\boxed{\mathbb{E}^x\left[e^{\frac{1}{\varepsilon} f(X_t^\varepsilon)}\right] = u^\varepsilon(T-t, x).}$$

$$\partial_t u^\varepsilon(t,x) + \frac{1}{\varepsilon}\sum_{j=1}^R \lambda_j^\varepsilon(x)\left[u^\varepsilon(t, x+\varepsilon\partial_j) - u^\varepsilon(t,x)\right]$$

$$u^\varepsilon(T,x) = e^{\frac{1}{\varepsilon} f(x)}$$

$$u^\varepsilon(t,x) = e^{\frac{1}{\varepsilon} S^\varepsilon(t,x)} \qquad S^\varepsilon(T,x) = f(x).$$

$$\frac{1}{\varepsilon}\partial_t S^\varepsilon(t,x)\, e^{\frac{1}{\varepsilon} S^\varepsilon(t,x)}$$

$$+ \frac{1}{\varepsilon}\sum_{j=1}^R \lambda_j^\varepsilon(x)\left[e^{\frac{1}{\varepsilon} S^\varepsilon(t, x+\varepsilon\partial_j)} - e^{\frac{1}{\varepsilon} S^\varepsilon(t,x)}\right] = 0$$

$$\Longleftrightarrow \quad \partial_t S^\varepsilon(t,x) + \sum_{j=1}^R \lambda_j^\varepsilon(x)\left[e^{\frac{1}{\varepsilon}\left[S^\varepsilon(t,x+\varepsilon\partial_j) - S^\varepsilon(t,x)\right]} - 1\right] = 0$$

$$\Big\}\ \varepsilon \downarrow 0$$

$$v^{\varepsilon} \xrightarrow[\varepsilon \downarrow 0]{} v$$

$$\partial_t v(t,x) + \underbrace{\sum_{j=1}^{R} \lambda_j(x)\left[e^{\gamma_j \cdot \nabla v(t,x)} - 1\right]}_{H(x,\nabla v)} = 0$$

$\boxed{\text{HJBE}}$

$$\begin{cases} \dot{x}_t = \partial_\theta H(x_t, \theta_t) = \displaystyle\sum_{j=1}^{R} \lambda_j(x_t)\, \gamma_j \, e^{\gamma_j \cdot \theta_t} \\[2ex] \dot{\theta}_t = -\partial_x H(x_t, \theta_t) = -\displaystyle\sum_{j=1}^{R} \nabla \lambda_j(x_t)\left[e^{\gamma_j \cdot \theta_t} - 1\right] \end{cases}$$

$\theta_{t} = 0 \longrightarrow$ LLN.

$$\dot{x}_t = \partial_\theta H(x_t, \theta_t = 0)$$

! H NOT quadratic + quadratic approx of $H \neq$ CLT.

ex: 1. Schlögl:

$$\lambda_+^{\varepsilon}(x) = k_0 + k_1 x(x-\varepsilon) \qquad \nu^+ = +1$$

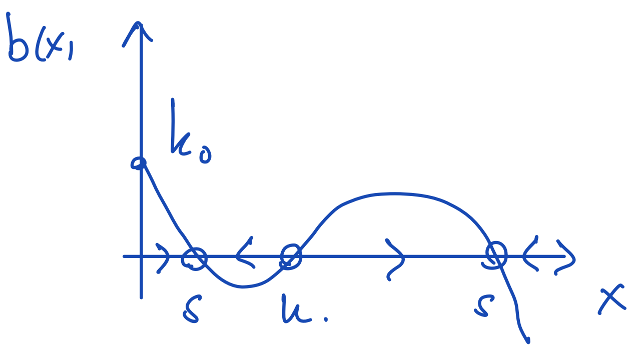
$$\lambda_-^{\varepsilon}(x) = k_1 x + k_3 x(x-\varepsilon)(x-2\varepsilon) \qquad \nu^- = -1$$

$$H(x,\theta) = (k_0 + k_1 x^2)(e^{\theta} - 1) + (k_1 x + k_3 x^3)(e^{-\theta} - 1)$$

$$\begin{cases} \dot{x}_t = (k_0 + k_1 x_t^2)\, e^{\theta_t} - (k_1 x_t + k_3 x_t^3)\, e^{-\theta_t} \\ \dot{\theta}_t = 2k_1 x^2 (e^{\theta_t} - 1) + (k_1 + 3k_3 x^2)(e^{-\theta_t} - 1) \end{cases}$$

@ $\theta_t = 0$

$$\dot{x}_t = \underbrace{k_0 + k_1 x_t^2 - k_1 x_t + k_3 x_t^3}_{= b(x_t)}$$



law of mass action

2. discrete diffusion :

$$H(x,\theta) = \alpha \sum_{j=1}^{M} \Big[x^j \left(e^{\theta_{j+1} - \theta_j} - 1 \right) + x^j \left(e^{\theta_{j-1} - \theta_j} - 1 \right) \Big]$$

$$= \alpha \sum_{j=1}^{M} x^j \left[e^{\theta_{j+1} - \theta_j} + e^{\theta_{j-1} - \theta_j} - 2 \right]$$

$$\boxed{\begin{aligned} \dot{x}^i_t &= \partial_{\theta_i} H = 2\alpha \Big[x^{i-1}_t e^{\theta^i_t - \theta^{i-1}_t} - x^i e^{\theta^{i+1}_t - \theta^i_t} + x^{i+1}_t e^{\theta^i_t - \theta^{i+1}_t} - x^i_t e^{\theta^{i-1}_t - \theta^i_t} \Big] \\ \dot{\theta}^i_t &= -\partial_{x_i} H = -\alpha \left(e^{\theta_{i+1} - \theta_i} + e^{\theta_{i-1} - \theta_i} - 2 \right) \end{aligned}}$$

LLN : $\dot{x}^i_t = 2\alpha \left[x^{i+1}_t + x^{i-1}_t - 2x^i_t \right]$

discrete diff eq.

NB continuous limit

$\vartheta_j = \vartheta(j\Delta s) \to \vartheta(s)$

$$e^{\vartheta_{j-1}-\vartheta_j} - 1 = e^{-h\,\partial_s\vartheta + \frac{h^2}{2}\partial_s^2\vartheta + \dots} - 1$$

$$= -h\,\partial_s\vartheta + \frac{h^2}{2}\left(\partial_s^2\vartheta + |\partial_s\vartheta|^2\right) + \dots$$

$$e^{\vartheta_{j+1}-\vartheta_j} = e^{+h\,\partial_s\vartheta + \frac{h^2}{2}\partial_s^2\vartheta + \dots}$$

$$= h\,\partial_s\vartheta + \frac{h^2}{2}\left(\partial_s^2\vartheta + |\partial_s\vartheta|^2\right)$$

$$\boxed{\sim\ \mathcal{H}(x,\vartheta) = 2\alpha\int_0^1 ds\ x(s)\left[\partial_s^2\vartheta + |\partial_s\vartheta|^2\right].}$$

$$\boxed{\begin{cases} \partial_t x(s) = \dfrac{\delta\mathcal{H}}{\delta\vartheta(s)} = 2\alpha\,\partial_s^2 x_t(s) - 2\alpha\,\partial_s\left(x_t(s)\,\partial_s\vartheta_t(s)\right) \\[2ex] \partial_t\vartheta(s) = -\dfrac{\delta\mathcal{H}}{\delta x(s)} = -2\alpha\left[\partial_s^2\vartheta_t(s) + |\partial_s\vartheta_t(s)|^2\right] \end{cases}}$$

NB: Another derivation:

$$dX_t^i = b(X_t^i)\,dt + \frac{1}{N}\sum_{j=1}^N c(X_t^i, X_t^j)\,dt + \sqrt{2D}\,dW_t^i .$$

$$\rho_N(t,x) = \frac{1}{N}\sum_{i=1}^N \delta(x - X_t^i)$$ empirical measure

$$d\rho_N(t,x) = -\frac{1}{N}\sum_{i=1}^N \nabla\delta(x - X_t^i)\cdot dX_t^i$$

$$+ \frac{D}{N}\sum_{i=1}^N \Delta\,\delta(x - X_t^i)\,dt$$

$$= -\frac{1}{N}\sum_{i=1}^N \nabla\delta(x - X_t^i)\cdot\Big(b(X_t^i) + \frac{1}{N}\sum_{j=1}^N c(X_t^i, X_t^j)\Big)dt$$

$$+ \frac{D}{N}\sum_{i=1}^N \Delta\,\delta(x - X_t^i)\,dt$$

$$- \frac{\sqrt{2D}}{N}\sum_{i=1}^N \nabla\delta(x - X_t^i)\cdot dW_t^i$$

$$\boxed{\begin{aligned} d\rho_N(t,x) = &-\nabla\cdot\Big[\Big(b(x) + \int c(x,y)\,\rho_N(t,y)\,dy\Big)\,\rho_N(t,x)\Big]\,dt \\ &+ D\,\Delta\rho_N(t,x)\,dt \\ &- \frac{\sqrt{2D}}{N}\sum_{i=1}^N \nabla\delta(x - X_t^i)\,dW_t^i . \end{aligned}}$$

$$\lim_{t \downarrow 0} \frac{1}{t} \mathbb{E}^{\rho_N^0} \left(\Phi[\rho_N(t)] - \Phi[\rho_N^0] \right)$$

$$= - \int \nabla \cdot \left[\left(b(x) + \int c(x,y) \rho_N^0(y) \, dy \right) \rho_N^0(x) \right] \frac{\delta \Phi}{\delta \rho_N^0(x)} \, dx$$

$$+ \int D \, \Delta \rho_N^0 \frac{\delta \Phi}{\delta \rho_N^0(x)}$$

$$+ \frac{D}{N^2} \sum_{i,j=1}^{N} \int \delta_{ij} \nabla_x \delta(x - x_0^i) \cdot \nabla_y \delta(y - x_0^j) \frac{\delta^2 \Phi}{\delta \rho_N^0(x) \, \delta \rho_N^0(y)} \, dx \, dy$$

//

$$\frac{D}{N} \sum_{i=1}^{N} \int \nabla_x \delta(x - x_0^i) \cdot \nabla_y \delta(y - x_0^i) \frac{\delta^2 \Phi}{\delta \rho_N^0(x) \, \delta \rho_N^0(y)} \, dx \, dy$$

$$= \frac{D}{N} \int \rho_N^0(x) \, \delta(x-y) \, \nabla_x \cdot \nabla_y \frac{\delta^2 \Phi}{\delta \rho_N^0(x) \, \delta \rho_N^0(y)} \, dx \, dy.$$

$$\Rightarrow \quad \boxed{\begin{aligned} H(\rho,\theta) = & \int \nabla\theta(x)\cdot\Big(b(x) + \int c(x,y)\,\rho(y)\,dy\Big)\rho(x)\,dx \\ & + D\int \Delta\theta(x)\,\rho(x)\,dx + D\int |\nabla\theta|^2\rho(x)\,dx \end{aligned}}$$

$$\boxed{\begin{aligned} \partial_t\rho_t(x) &= \frac{\delta H}{\delta\theta(x)} = -\nabla\cdot\Big[\Big(b(x) + \int c(x,y)\,\rho_t(y)\Big)\rho_t(x)\Big] \\ &\qquad + D\,\Delta\rho_t(x) - 2\,\nabla\cdot\big(\rho_t(x)\,\nabla\theta_t(x)\big) \\ \partial_t\theta_t(x) &= -\frac{\delta H}{\delta\rho(x)} = -b(x)\cdot\nabla\theta_t(x) - \int c(y,x)\,\nabla\theta_t(y)\,\rho_t(y)\,dy \\ &\qquad - D\,\Delta\theta_t(x) - D\,|\nabla\theta_t(x)|^2 \end{aligned}}$$