Gradient structures and discrete Markov chain models for reaction-diffusion systems

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From Particle Systems to Differential Equations

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Partial support via "*Analysis of multiscale dystems driven by functionals*"

Overview

1. Introduction
2. Markov chains as gradient systems
3. Reaction-diffusion systems as gradient systems
4. Discrete-to-continuum passage
5. Limit of chemical master equations
6. Coupling reaction and diffusion

Semiconductor model: van Roosbroeck system

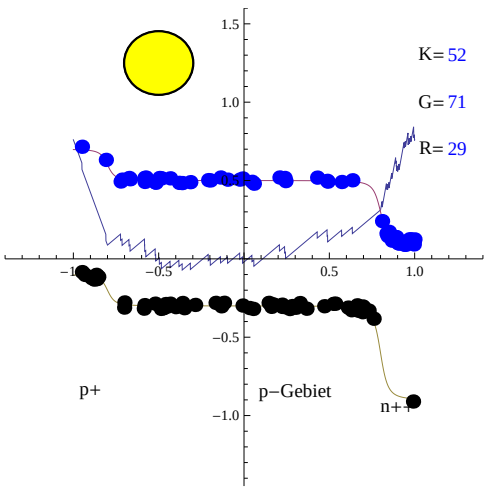
$$-\operatorname{div}(\varepsilon\nabla\phi) = d - n + p \qquad \text{electrostatics}$$

$$\dot{n} = \operatorname{div}\left(\mu_n(\nabla n - n\nabla\phi)\right) + g - rnp \qquad \text{electron balance}$$

$$\dot{p} = \operatorname{div}\left(\mu_p\left(\nabla p + p\nabla\phi\right)\right) + g - rnp \qquad \text{hole balance}$$

Motivation:

- understand the van Roosbroeck system as the limit of a many-particle system
- learn how to model diffusion in random media (organic semiconductors)



1. Introduction

particle system	$\rightsquigarrow$	differential equation
random walk	$\rightsquigarrow$	diffusion equation
$\dot{u}_m = \mu M^2 \big(u_{m-1} - 2u_m + u_{m+1}\big)$		$\dot{U} = \mu \Delta U$
chemical master equations	$\rightsquigarrow$	reaction kinetic
$\dot{u}_n = \gamma u_{n-1} + \alpha \frac{n^p}{N^p} u_{n+1} - (...) u_n$		$\dot{U} = \gamma - \alpha U^p$
Markov chain		ODEs / PDEs

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Main philosophy: Use gradient structure $\dot{\boldsymbol{u}} = -\mathcal{K}(\boldsymbol{u})\mathrm{D}\mathcal{E}(\boldsymbol{u})$

$(\mathcal{X}, \mathcal{E}, \mathcal{K})$ gradient system

$\mathcal{X}$ state space containing the states $\boldsymbol{u} \in \mathcal{X}$.

$\mathcal{E} : \mathcal{X} \to \mathbb{R}$ energy functional with differential $\mathrm{D}\mathcal{E}(\boldsymbol{u}) \in \mathsf{T}^*_{\boldsymbol{u}}\mathcal{X}$

$\mathcal{G}(\boldsymbol{u})^{-1} = \mathcal{K}(u) : \mathsf{T}^*_{\boldsymbol{u}}\mathcal{X} \to \mathsf{T}_{\boldsymbol{u}}\mathcal{X}$ inverse of metric: Onsager oper. $\mathcal{K} = \mathcal{K}^* \geq 0$

1. Introduction

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Study discrete-to-continuum limit for gradient structures

$\boldsymbol{u}^\varepsilon$ solves $(\mathcal{X}, \mathcal{E}_\varepsilon, \mathcal{K}_\varepsilon)$ discrete model $\varepsilon = \frac{1}{N}$, $N = \#$ particles

$$\Downarrow$$

$\boldsymbol{u}$ solves $(\mathcal{X}, \mathcal{E}, \mathcal{K})$ continuum model

We want to conclude $\boldsymbol{u}^\varepsilon(t) \to \boldsymbol{u}(t)$ from $(\mathcal{E}_\varepsilon, \mathcal{K}_\varepsilon) \rightsquigarrow (\mathcal{E}, \mathcal{K})$!!

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2. Markov chains as gradient systems

- Otto 1999: Fokker-Planck equation $\dot{U} = \operatorname{div}\big(\nabla U + U\nabla V\big)$ is a gradient system $(\mathcal{X}, \mathcal{E}, \mathcal{K})$:

$\mathcal{E}(U) = \int_\Omega U \log(U/W)$ with $W(x) = c\mathrm{e}^{-V(x)}$ $\quad \rightsquigarrow \mathrm{D}\mathcal{E}(U) = \log U + V$

$\mathcal{K}(U)\xi = -\operatorname{div}(U\nabla\xi)$ $\quad \rightsquigarrow \dot{U} = -\mathcal{K}(U)\mathrm{D}\mathcal{E}(U)$

- M'10: Reaction-diffusion systems satisfying the detailed-balance condition (and possibly including temperature or drift due to electric charges) have a gradient structure for the relative entropy.

- Maas'11, M'11: Discrete Markov chains with detailed-balance condition have a gradient structure for the relative entropy.

2. Markov chains as gradient systems

Discrete Markov chain on states $j \in J$ (e.g. $\mathbb{Z}_M^d$ or $\mathbb{N}_0^m$)

$\mathcal{X} = \mathsf{Prob}(J) = \{\, \boldsymbol{u} = (u_j)_{j\in J} \in \ell^1(J) \,|\, u_j \geq 0,\ \sum_J u_j = 1 \,\}$

$\dot{\boldsymbol{u}} = Q\boldsymbol{u}$ linear evolution with unique steady state $\boldsymbol{w} = (w_j)_J$

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Theorem (M'11, Maas'11).

If Q satisfies the **detailed balance condition (DBC)**

$$w_j > 0 \text{ and } Q_{jk}w_k = Q_{kj}w_j \text{ for all } j,k \in J,$$

then we have the gradient structure $\dot{\boldsymbol{u}} = Q\boldsymbol{u} = -\mathcal{K}_{\mathsf{Mv}}(\boldsymbol{u})\mathrm{D}\mathcal{E}(\boldsymbol{u})$

with $\mathcal{E}(\boldsymbol{u}) = \sum_J u_j \log(u_j/w_j)$ and

$$\mathcal{K}_{\mathsf{Mv}}(\boldsymbol{u}) = \sum_{j,k\in J} \frac{1}{2} Q_{jk}w_k\, \Lambda\Big(\frac{u_j}{w_j}, \frac{u_k}{w_k}\Big)\, \mathbb{E}_{jk} \ \in \mathbb{R}^{J\times J}_{\geq 0} \text{ where}$$

$\mathbb{E}_{jk} = \mathbb{E}_{jk}^* = (e_j - e_k) \otimes (e_j - e_k) \geq 0$ and $\Lambda(a,b) = \frac{a-b}{\log(a/b)} \geq 0.$

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$\mathbb{E}_{jk} = \mathbb{E}_{jk}^* = (e_j - e_k) \otimes (e_j - e_k) \geq 0$ and $\Lambda(a,b) = \frac{a-b}{\log(a/b)} \geq 0.$

To be proved: $\dot{\boldsymbol{u}} = Q\boldsymbol{u} = -\mathcal{K}_{\mathsf{Mv}}(\boldsymbol{u}) \mathsf{D}\mathcal{E}(\boldsymbol{u})$

- $\mathsf{D}\mathcal{E}(\boldsymbol{u}) = (\log(u_j/w_j) + 1)_J \quad \Longrightarrow$

$$\mathbb{E}_{jk} \mathsf{D}\mathcal{E}(\boldsymbol{u}) = \big(\log(u_j/w_j) - \log(u_k/w_k)\big) \, (e_j - e_k)$$

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  $\mathbb{E}_{jk} \mathsf{D}\mathcal{E}(\boldsymbol{u}) = \big(\log(u_j/w_j) - \log(u_k/w_k)\big) \, \big(e_j - e_k\big)$
- Using the cancellation $\Lambda(a,b)\big(\log a - \log b\big) = (a-b)$ gives
  $\mathcal{K}_{\mathsf{Mv}}(\boldsymbol{u}) \mathsf{D}\mathcal{E}(\boldsymbol{u}) = \sum_{j,k\in J} \frac{Q_{jk} w_k}{2} \, \big(\frac{u_j}{w_j} - \frac{u_k}{w_k}\big) \, \big(e_j - e_k\big)$ (already linear)
- Using detailed balance gives $\mathcal{K}_{\mathsf{Mv}}(\boldsymbol{u}) \mathsf{D}\mathcal{E}(\boldsymbol{u}) = -Q\boldsymbol{u}$.

QED

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3. Reaction-diffusion systems as gradient systems

$\boldsymbol{u} = (u_1(t,x), ..., u_I(t,x))$ densities of chemical species

Reaction-diffusion systems $\dot{\boldsymbol{u}} = \operatorname{div}\big(M(\boldsymbol{u})\nabla \boldsymbol{u}\big) + \boldsymbol{R}(\boldsymbol{u})$

Example: Ammonia synthesis

$\mathsf{N}_2 + 3H_2 \rightleftharpoons 2\mathsf{NH}_3 \qquad \boldsymbol{u} = (u_{\mathsf{N}_2}, u_{\mathsf{H}_2}, u_{\mathsf{NH}_3}) = (u_1, u_2, u_3)$

$$\begin{pmatrix} \dot{u}_1 \\ \dot{u}_2 \\ \dot{u}_3 \end{pmatrix} = \begin{pmatrix} m_1\Delta u_1 \\ m_2\Delta u_2 \\ m_3\Delta u_3 \end{pmatrix} + \underbrace{\begin{pmatrix} -(k_{\mathsf{f}} u_1 u_2^3 - k_{\mathsf{b}} u_3^2) \\ -3(k_{\mathsf{f}} u_1 u_2^3 - k_{\mathsf{b}} u_3^2) \\ +2(k_{\mathsf{f}} u_1 u_2^3 - k_{\mathsf{b}} u_3^2) \end{pmatrix}}_{=\boldsymbol{R}(\boldsymbol{u})}$$

The usual guess of Allen-Cahn or Cahn-Hillard type

$\mathcal{E}(\boldsymbol{u}) = \int_\Omega m_1|\nabla u_1|^2 + m_2|\nabla u_2|^2 + m_3|\nabla u_3|^2 + F(\boldsymbol{u})\,\mathrm{d}x$ does NOT work,

since curl $\boldsymbol{R} \not\equiv 0$!

3. Reaction-diffusion systems as gradient systems

Reaction-diffusion systems (RDS) $\qquad \dot{\boldsymbol{u}} = \mathrm{div}\left(M(\boldsymbol{u})\nabla \boldsymbol{u}\right) + \boldsymbol{R}(\boldsymbol{u})$

Reaction kinetic of mass-action type with detailed balance cond. (DBC)

$$\dot{\boldsymbol{u}} = \boldsymbol{R}(\boldsymbol{u}) = -\sum_{r=1}^{R} k_r \left(\underbrace{\frac{\boldsymbol{u}^{\boldsymbol{\alpha}^r}}{\boldsymbol{w}^{\boldsymbol{\alpha}^r}}}_{\text{educts}} - \underbrace{\frac{\boldsymbol{u}^{\boldsymbol{\beta}^r}}{\boldsymbol{w}^{\boldsymbol{\beta}^r}}}_{\text{products}} \right) \underbrace{\left(\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r \right)}_{\text{stoich. vect.}} \qquad \boldsymbol{u}^{\boldsymbol{\gamma}} = \prod_{i=1}^{I} u_i^{\gamma_i}$$

(DBC = for $\boldsymbol{u} = \boldsymbol{w}$ each reaction $r = 1, ..., R$ is balanced)

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Gradient structure for reaction kinetics: $\dot{\boldsymbol{u}} = \boldsymbol{R}(\boldsymbol{u}) = -\mathbb{K}(\boldsymbol{u})\mathrm{D}E(\boldsymbol{u})$

$E(\boldsymbol{u}) = \sum_i^I u_i \log(u_i/w_i)$ and

$$\mathbb{K}(\boldsymbol{u}) = \sum_{r=1}^{R} k_r \, \Lambda\left(\frac{\boldsymbol{u}^{\boldsymbol{\alpha}^r}}{\boldsymbol{w}^{\boldsymbol{\alpha}^r}}, \frac{\boldsymbol{u}^{\boldsymbol{\beta}^r}}{\boldsymbol{w}^{\boldsymbol{\beta}^r}}\right) \left(\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r\right) \otimes \left(\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r\right) \ \in \mathbb{R}^{I\times I}_{\geq 0}$$

with $\Lambda(a,b) = \frac{a-b}{\log a - \log b} > 0$ $\qquad$ [use again $\boldsymbol{\gamma} \cdot (\log v_i) = \log(\boldsymbol{v}^{\boldsymbol{\gamma}})$]

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(DBC = for $\boldsymbol{u} = \boldsymbol{w}$ each reaction $r = 1, ..., R$ is balanced)

Gradient structure for RDS with DBC: $\boxed{\dot{\boldsymbol{u}} = -\mathcal{K}_{\mathsf{RDS}}(\boldsymbol{u})\mathsf{D}\mathcal{E}(\boldsymbol{u})}$

$$\mathcal{E}(\boldsymbol{u}) = \int_\Omega E(\boldsymbol{u}(x))\,\mathrm{d}x = \int_\Omega u_i(x)\log(u_i(x)/w_i(x))\,\mathrm{d}x$$

$$\mathcal{K}_{\mathsf{RDS}}(\boldsymbol{u})\boldsymbol{\xi} = \underbrace{-\operatorname{div}\big(\mathbb{M}(\boldsymbol{u})\nabla\boldsymbol{\xi}\big)}_{\text{diffusion}} + \underbrace{\mathbb{K}(\boldsymbol{u})\xi}_{\text{react}}$$

Onsager'31: $\mathbb{K} = \mathbb{K}^* \geq 0$ and $\mathbb{M} = \mathbb{M}^* \geq 0$ mobilities

$M(\boldsymbol{u}) = \mathbb{M}(\boldsymbol{u})\mathsf{D}^2 E(\boldsymbol{u}) = \mathbb{M}(\boldsymbol{u})\mathrm{diag}(\frac{1}{u_1}, ..., \frac{1}{u_I})$ not necess. symm.

Example: Ammonia synthesis $\mathsf{N}_2 + 3H_2 \leftrightharpoons 2\mathsf{NH}_2$

$$\begin{pmatrix} \dot u_1 \\ \dot u_2 \\ \dot u_3 \end{pmatrix} = \begin{pmatrix} m_1\Delta u_1 \\ m_2\Delta u_2 \\ m_3\Delta u_3 \end{pmatrix} + \begin{pmatrix} -(k_\mathsf{f} u_1 u_2^3 - k_\mathsf{b} u_3^2) \\ -3(k_\mathsf{f} u_1 u_2^3 - k_\mathsf{b} u_3^2) \\ +2(k_\mathsf{f} u_1 u_2^3 - k_\mathsf{b} u_3^2) \end{pmatrix}$$

- reference density $\boldsymbol{w} = (k_\mathsf{b}, k_\mathsf{f}, k_\mathsf{f}^2)$
- relative entropy

$$\mathcal{E}(\boldsymbol{u}) = \int_\Omega u_1 \log(u_1/w_1) + u_2 \log(u_2/w_2) + u_3 \log(u_3/w_3)\,\mathrm{d}x$$

- Onsager operator

$$\mathcal{K}_{\mathsf{RDS}}(\boldsymbol{u})\boldsymbol{\xi} = -\begin{pmatrix} m_1\,\mathsf{div}(u_1\nabla\xi_1) \\ m_2\,\mathsf{div}(u_2\nabla\xi_2) \\ m_3\,\mathsf{div}(u_3\nabla\xi_3) \end{pmatrix} + \Lambda\Big(\tfrac{u_1u_2^3}{w_1w_2^3}, \tfrac{u_3^2}{w_2^3}\Big) \begin{pmatrix} 1 & 3 & -2 \\ 3 & 9 & -6 \\ -2 & -6 & 4 \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \end{pmatrix}$$

Semiconductor model: van Roosbroeck system

$$-\operatorname{div}(\varepsilon\nabla\phi) = d - n + p \qquad \text{electrostatics}$$

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Gradient structure[1] $(\dot{n},\dot{p}) = -\mathcal{K}_{\mathsf{vR}}(n,p)\mathsf{D}\mathcal{E}(n,p)$

[1] M.: Grad. structures for RDS and energy-drift-diffusion systems, Nonlin. 2011

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Gradient structure[1] $(\dot n, \dot p) = -\mathcal{K}_{\mathsf{vR}}(n,p)\mathrm{D}\mathcal{E}(n,p)$

- Reference density $\boldsymbol{w} = (w, w)$ with $w = (g/r)^{1/2}$
- Free energy $\mathcal{E}_{\mathsf{vR}}(n,p) = \int_\Omega n\log(n/w) + p\log(p/w) + \frac{\varepsilon}{2}|\nabla\phi_{n,p}|^2\,\mathrm{d}x$
- Onsager oper. $\mathcal{K}_{\mathsf{vR}}(n,p)\binom{\xi_n}{\xi_p} = -\binom{\operatorname{div}(n\mu_n\nabla\xi_n)}{\operatorname{div}(p\mu_p\nabla\xi_p)} + g\Lambda\big(1, \frac{np}{w^2}\big)\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}\binom{\xi_n}{\xi_p}$

Crucial observation (AlbGajHün'01) $\mathrm{D}\mathcal{E}_{\mathsf{vR}} = \binom{\log(n/w)+1}{\log(p/w)+1} + \phi_{n,p}\binom{-1}{+1}$

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- already very well understood with many approaches
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State space $J = \mathbb{Z}_M = \mathbb{Z}/_{M\mathbb{Z}}$

$\dot{u}_m = \mu M^2(u_{m-1} - 2u_m + u_{m+1}) \qquad \dot{\boldsymbol{u}} = Q\boldsymbol{u} = -\mathcal{K}^M(\boldsymbol{u})\mathsf{D}\mathcal{E}^M(\boldsymbol{u})$

- $\mathcal{E}^M(\boldsymbol{u}) = \sum_1^M u_i \log(Mu_i)$ where $\boldsymbol{w} = \frac{1}{M}(1, ..., 1)$ and
- $\mathcal{K}^M(\boldsymbol{u}) = \sum_1^M \mu M^2 \Lambda(u_m, u_{m+1})\mathbb{E}_{m,m+1} \geq 0$ (tridiagonal)

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Riemannian transport distance on $\mathcal{X}^M = \mathsf{Prob}(\mathbb{Z}_M)$

$d_{\mathcal{K}^M} : \mathcal{X}^M \times \mathcal{X}^M \to [0, \infty[$ defined via

$$d_{\mathcal{K}^M}(\boldsymbol{u}_0, \boldsymbol{u}_1)^2 = \inf\Big\{ \int_0^1 u'(s) \cdot \underbrace{\mathcal{K}^M(\boldsymbol{u}(s))^{-1}}_{\text{Riemannian tensor}} \boldsymbol{u}'(s)\,\mathrm{d}s \;\Big|\; \boldsymbol{u}_0 \overset{\boldsymbol{u}}{\rightsquigarrow} \boldsymbol{u}_1 \Big\}.$$

Markov chain is metric gradient flow $(\mathcal{X}^M, \mathcal{E}^M, d_{\mathcal{K}^M})$ in De Giorgi's sense!

4. Discrete-to-continuum passage

$\dot u_m = \mu M^2(u_{m-1} - 2u_m + u_{m+1})$, $m \in \mathbb{Z}_M$ $\qquad$ $\dot{\boldsymbol{u}} = -\mathcal{K}^M(\boldsymbol{u})\mathsf{D}\mathcal{E}^M(\boldsymbol{u})$

Limit passage: embed $\mathcal{X}^M = \mathsf{Prob}(\mathbb{Z}_M)$ into $\mathcal{X} = \mathsf{Prob}(\mathbb{S}^1)$

$U = I_M \boldsymbol{u}$ with $U(x) = \sum_{m=1}^M M u_m \chi_{](m-1)/M, m/M]}(x)$

$\dot u_m = \mu M^2(u_{m-1} - 2u_m + u_{m+1})$ $\xrightarrow{\text{to be shown}}$ $\dot U = \mu U_{xx}$

4. Discrete-to-continuum passage

$$\dot u_m = \mu M^2(u_{m-1} - 2u_m + u_{m+1}),\ m \in \mathbb{Z}_M \qquad \dot{\boldsymbol{u}} = -\mathcal{K}^M(\boldsymbol{u})\mathsf{D}\mathcal{E}^M(\boldsymbol{u})$$

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$\dot u_m = \mu M^2(u_{m-1} - 2u_m + u_{m+1})$ $\xrightarrow{\text{to be shown}}$ $\dot U = \mu U_{xx}$

$\mathcal{E}^M(\boldsymbol{u}) = \sum_1^M u_i \log(Mu_i)$ $\xrightarrow{\text{trivial via } I_M}$ $\mathcal{E}(U) = \int_0^1 U \log U \,\mathrm{d}x$

$\boldsymbol{\xi}\cdot\mathcal{K}^M(\boldsymbol{u})\boldsymbol{\xi} =$ $\qquad$ $\langle \Xi, \mathcal{K}(U)\Xi\rangle =$

$\sum_1^M \mu\Lambda(u_m, u_{m+1})M^2(\xi_m - \xi_{m+1})^2$ $\xrightarrow{\text{in what sense?}}$ $\int_0^1 \mu U|\Xi'|^2 \,\mathrm{d}x$

- formally $\mathcal{K}^M(\boldsymbol{u}) \rightsquigarrow \mathcal{K}(U)$ as quadratic forms
- but in what sense do we need convergence to guarantee convergence of solutions?

4. Discrete-to-continuum passage

Limit passage: $\dot{u}_m = \mu M^2(u_{m-1} - 2u_m + u_{m+1}) \xrightarrow{\text{to be shown}} \dot{U} = \mu U_{xx}$

Use metric approach instead:

Evolutionary variational inequality (EVI) (cf. Ambrosio,Gigli,Savaré'05)

If $\mathcal{E}$ is geodesically convex with respect to $d_{\mathcal{K}}$, then

$$\dot{\boldsymbol{u}} = -\mathcal{K}(\boldsymbol{u})\mathrm{D}\mathcal{E}(\boldsymbol{u}) \quad \Longleftrightarrow \quad \text{(EVI)} \quad \tfrac{\mathrm{d}^+}{\mathrm{d}t} d(\boldsymbol{u}(t), \boldsymbol{v})^2 + \mathcal{E}(\boldsymbol{u}(t)) \le \mathcal{E}(\boldsymbol{v})$$

for all $t \ge 0$ and $\boldsymbol{v} \in \mathcal{X}$

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If $\mathcal{E}$ is geodesically convex with respect to $d_{\mathcal{K}}$, then

$$\dot{\boldsymbol{u}} = -\mathcal{K}(\boldsymbol{u})\mathsf{D}\mathcal{E}(\boldsymbol{u}) \iff \text{(EVI)} \quad \frac{\mathrm{d}^+}{\mathrm{d}t} d(\boldsymbol{u}(t), \boldsymbol{v})^2 + \mathcal{E}(\boldsymbol{u}(t)) \le \mathcal{E}(\boldsymbol{v})$$

for all $t \ge 0$ and $\boldsymbol{v} \in \mathcal{X}$

Theorem M'12.
If $(\mathcal{X}^M, \mathcal{E}^M, d_{\mathcal{K}^M})$ and $(\mathcal{X}, \mathcal{E}, d_{\mathsf{W}})$ are given as above, then

$$I_M \boldsymbol{u}^M(0) \overset{d_{\mathsf{W}}}{\to} U(0) \implies I_M \boldsymbol{u}^M(t) \overset{d_{\mathsf{W}}}{\to} U(t) \text{ for all } t \ge 0.$$

- M.11: $(\mathcal{X}^M, \mathcal{E}^M, d_{\mathcal{K}^M})$ is geodesically 0-convex (indep. of M)
- Gigli-Maas'11/12: $d_{\mathsf{W}} = \Gamma\text{-}\lim_{M\to\infty} d_{\mathcal{K}^M}$
- Use EVI and $\mathcal{E} = \Gamma\text{-}\lim_{M\to\infty} \mathcal{E}^M$.

Overview

1. Introduction
2. Markov chains as gradient systems
3. Reaction-diffusion systems as gradient systems
4. Discrete-to-continuum passage
5. **Limit of chemical master equations**
6. Coupling reaction and diffusion

5. Limit of chemical master equations

Simple reaction equation $\dot{a} = 1 - a^p$ (1=generation, $-a^p$ annihilation)

Gradient system $([0,\infty[\,, a\log a - a, \mathbb{K})$ with $\mathbb{K}(a) = \Lambda(1, a^p)p$

Chemical master equation: keep track of number of particles!

$a = \frac{1}{N}\,\#$ number of particles, where $N =$ typical number of particles

$u_n =$ probability of having exactly n particles

Markov chain: $\dot{u}_n = \underbrace{1\,u_{n-1}}_{\text{generation}} - \underbrace{\big(1 + (\tfrac{n}{N})^p\big)u_n}_{\text{losses}} + \underbrace{(\tfrac{n+1}{N})^p u_{n+1}}_{\text{annihilation}}$

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- DBC holds for $\boldsymbol{w}^N = (w_n^N)$ with $w_n^N = \big(\frac{N^n}{n!}\big)^p w_0^N$
- We have the gradient structure $(\mathcal{X}_{\mathsf{CME}}, \mathcal{E}^N, \mathcal{K}^N)$ with
  - $\mathcal{X}_{\mathsf{CME}} = \{\, \boldsymbol{u} \in \ell_1(\mathbb{N}_0) \mid u_n \ge 1, \|\boldsymbol{u}\|_1 = 1 \,\}$
  - $\mathcal{E}^N(\boldsymbol{u}) = \sum_{n=0}^\infty u_n \log(u_n/w_n^N)$
  - $\mathcal{K}^N(\boldsymbol{u}) = \sum_{n=1}^\infty w_{n-1}^N \Lambda\big(\frac{u_{n-1}}{w_{n-1}^N}, \frac{u_n}{w_n^N}\big)\mathbb{E}_{n-1,n} \ \ge 0$

5. Limit of chemical master equations

Limit passage $N \to \infty$

We embed $\mathcal{X}_{\mathsf{CME}}$ into Prob$([0,\infty[)$ via

$U = I_N \boldsymbol{u}$ with $U(a) = \sum_{n=1}^{M} N\, u_n\, \chi_{](n-1)/N, n/N]}(a)$ $\qquad$ "$a \approx n/N$"

We use the expansion (large deviation argument)

$-\frac{1}{N} \log w_n^N \;\approx\; E(n/N)$ where $E(a) = p(a \log a - a + 1)$ $\quad$ (rate fcn.)

$\rightsquigarrow \mathcal{E}^N(\boldsymbol{u}) \approx \sum_0^\infty \big(u_n \log u_n + N u_n E(n/N)\big)$

We find Γ-convergence $\frac{1}{N}\mathcal{E}^N \overset{\Gamma}{\to} \boldsymbol{E}$ where $\boldsymbol{E}(U) = \int_0^\infty U(a) E(a)\, \mathrm{d}a$

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Moreover,

$$\boldsymbol{\xi}\cdot N\mathcal{K}^N(\boldsymbol{u}^N)\boldsymbol{\xi} = \sum_1^\infty \underbrace{w_{n-1}^N \Lambda\big(\tfrac{u_{n-1}}{w_{n-1}^N}, \tfrac{u_n}{w_n^N}\big)}_{\approx U(n/N)\Lambda(1,(n/N)^p)} N^2(\xi_n - \xi_{n-1})^2 \tfrac{1}{N}$$

$$\xrightarrow{\text{formally}} \int_0^\infty U(a)\Lambda(1,a^p)(\Xi'(a))^2\,\mathrm{d}a$$

5. Limit of chemical master equations

Markov chain: $\dot{u}_n = u_{n-1} - \big(1 + (\frac{n}{N})^p\big)u_n + (\frac{n+1}{N})^p u_{n+1}$

Gradient structure $(\mathcal{X}, \mathcal{E}^N, \mathcal{K}^N)$ with

$\mathcal{X} = \{\, \boldsymbol{u} \in \ell_1(\mathbb{N}_0) \,|\, u_n \geq 1, \|\boldsymbol{u}\|_1 = 1 \,\}$

$\mathcal{E}^N(\boldsymbol{u}) = \sum_{n=0}^{\infty} u_n \log(u_n/w_n^N),$

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The embedding $(\mathrm{Prob}([0,\infty[), \mathcal{E}^N \circ I_N, \mathcal{K}^N \circ I_N)$ converges formally to the limiting gradient system $(\mathrm{Prob}([0,\infty[), \boldsymbol{E}, \boldsymbol{K})$ with

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Result: Liouville equation = transport equation (cf. T.R.Kurtz'67-70)

$\dot{U}(t,a) = -\big((1-a^p)U(t,a)\big)'$ since $\mathrm{D}\boldsymbol{E} = E$ and $K(a)E'(a) = a^p - 1$

5. Limit of chemical master equations

Inspired by Eindhoven group (Mark Peletier, Michiel Renger, ...)

A similar result holds for N-particle Markov chains

$\dot{\boldsymbol{u}} = Q\boldsymbol{u}$ single-particle process

$\boldsymbol{u} = (u_j)_{j\in J} \in \mathsf{Prob}(J), \quad \mathcal{E}_{\mathsf{MV}}(\boldsymbol{u}) = \sum_{j\in J} u_j \log(u_j/w_j)$

N independent particles: $\dot{\mathbb{U}} = \frac{1}{N}\mathbb{Q}^N\mathbb{U}$ (time rescaling)

$\mathbb{U} = (\mathbb{U}_{\boldsymbol{n}})_{\boldsymbol{n}\in\mathbb{J}_N} \in \mathsf{Prob}(\mathbb{J}_N)$ where $\mathbb{J}_N = \{\, \boldsymbol{n} \in \mathbb{N}_0^J \mid \sum_{j\in J} n_j = N \,\}$

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Lemma If $\dot{\boldsymbol{u}} = Q\boldsymbol{u}$ satisfies DBC for $\boldsymbol{w}$, then $\dot{\mathbb{U}} = \frac{1}{N}\mathbb{Q}^N\mathbb{U}$ satisfies DBC for $\mathbb{W}$ with

$$\mathbb{W} = (\mathbb{W}_{\boldsymbol{n}})_{\boldsymbol{n}\in\mathbb{J}_N} \text{ with } \mathbb{W}_{\boldsymbol{n}} = N! \prod_{j\in J} w_j^{n_j}/(n_j!)$$

Gradient structure $(\mathrm{Prob}(\mathbb{J}_N), \mathbb{E}_N, \mathbb{K}_N)$ with $\mathbb{E}_N(\mathbb{U}) = \sum_{\boldsymbol{n}\in\mathbb{J}_N} \mathbb{U}_{\boldsymbol{n}} \log(\mathbb{U}_{\boldsymbol{n}}/\mathbb{W}_{\boldsymbol{n}})$

5. Limit of chemical master equations

Independence of particles gives a large-deviation result

$\frac{1}{N}\log \mathbb{W}_{\boldsymbol{n}} \approx -\mathcal{E}_{\mathsf{Mv}}(\frac{1}{N}\boldsymbol{n})$ $\leftarrow$ single-part. energy!

We again embed $\mathrm{Prob}(\mathbb{J}_N)$ into $\mathrm{Prob}(\underbrace{\mathrm{Prob}(J)}_{\text{Gibbs simplex}})$ via

$U = I_N\mathbb{U}$ where $U(\boldsymbol{u}) = \sum_{\boldsymbol{n}\in\mathbb{J}_N} \mathbb{U}_{\boldsymbol{n}} c^N \chi_0(\boldsymbol{u}-\frac{1}{N}\boldsymbol{n})$

As above $\quad \frac{1}{N}\mathbb{E}_N \circ I_N \xrightarrow{\Gamma} \boldsymbol{E}$ with $\boldsymbol{E}(U) = \int_{\mathrm{Prob}(J)} U(\boldsymbol{u})\mathcal{E}_{\mathsf{Mv}}(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u}$

$\mathbb{K}_N \xrightarrow{\text{formally}} \boldsymbol{K}$ with $\boldsymbol{K}(U) = -\operatorname{div}_{\boldsymbol{u}}\big(U\mathcal{K}_{\mathsf{Mv}}(\boldsymbol{u})\nabla_{\boldsymbol{u}}\xi\big)$

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Limiting system: Liouville equation = transport equation

$$\boxed{\dot{U}(t,\boldsymbol{u}) = -\operatorname{div}_{\boldsymbol{u}}\left(U(t,\boldsymbol{u})Q\boldsymbol{u}\right)}$$

since $\mathsf{D}_U\boldsymbol{E} = \mathcal{E}_{\mathsf{Mv}}$ and $-\boldsymbol{K}(U)\mathsf{D}\boldsymbol{E} = \operatorname{div}_{\boldsymbol{u}}(U\underbrace{\mathcal{K}_{\mathsf{Mv}}\mathsf{D}_{\boldsymbol{u}}\mathcal{E}_{\mathsf{Mv}}}_{=-Q\boldsymbol{u}}) = -\operatorname{div}_{\boldsymbol{u}}\left(UQ\boldsymbol{u}\right)$

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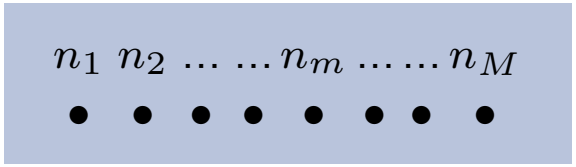
Open problem: Can we find similar PDE limits for a **Markov chain** coupling reaction and diffusion?

Attempt: Model $\dot{U} = \mu U_{xx} + 1 - U^2$



using $\mathbb{J}_{K,N} = \{\, \boldsymbol{n} = (n_1, .., n_M) \in \mathbb{N}_0^M \mid \sum_1^M n_m = KN \,\}$ and

$u_{\boldsymbol{n}} = u_{(n_1,...,n_M)}$ = prob. that site m has n_m part. $(m = 1, ..., M)$

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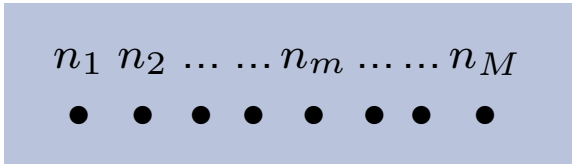

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Idea: model directly the gradient structure (instead of Markov chain)

$$\mathbb{E}_{M,N}(\mathbb{U}) = \sum_{\boldsymbol{n}\in\mathbb{J}_{M,N}} \mathbb{U}_{\boldsymbol{n}} \log\big(\mathbb{U}_{\boldsymbol{n}}/\mathbb{W}_{\boldsymbol{n}}\big) \text{ and } \mathbb{K} = \mathbb{K}_{\mathsf{diff}} + \mathbb{K}_{\mathsf{react}}$$

$$\boldsymbol{\xi}\cdot\mathbb{K}_{\mathsf{react}}(\mathbb{U})\boldsymbol{\xi} = \sum_{\boldsymbol{n}\in\mathbb{J}_{M,N}} \sum_{m=1}^{M} \rho_{m,\boldsymbol{n}}^{M,N} \mathbb{W}_{\boldsymbol{n}} \Lambda\big(\tfrac{\mathbb{U}_{\boldsymbol{n}}}{\mathbb{W}_{\boldsymbol{n}}}, \tfrac{\mathbb{U}_{\boldsymbol{n}+e_m}}{\mathbb{W}_{\boldsymbol{n}+e_m}}\big)(\xi_{\boldsymbol{n}} - \xi_{\boldsymbol{n}+e_m})^2$$

where $e_m = (0, .., 0, 1, 0..)$

$$\boldsymbol{\xi}\cdot\mathbb{K}_{\mathsf{diff}}(\mathbb{U})\boldsymbol{\xi} = \sum_{\boldsymbol{n}\in\mathbb{J}_{M,N}} \sum_{m=1}^{M} \mu_{m,\boldsymbol{n}}^{M,N} \mathbb{W}_{\boldsymbol{n}} \Lambda\big(\tfrac{\mathbb{U}_{\boldsymbol{n}}}{\mathbb{W}_{\boldsymbol{n}}}, \tfrac{\mathbb{U}_{\boldsymbol{n}+\delta_m}}{\mathbb{W}_{\boldsymbol{n}+\delta_m}}\big)(\xi_{\boldsymbol{n}} - \xi_{\boldsymbol{n}+\delta_m})^2$$

where $\delta_m = e_m - e_{m-1}$

Conclusion

- Markov chains and RDS with DBC have gradient structures
- The Onsager form $\dot{\boldsymbol{u}} = -\mathcal{K}(\boldsymbol{u})\mathrm{D}\mathcal{E}(\boldsymbol{u})$ allows for easy modeling

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Thank you for your attention

WIAS preprints at http://www.wias-berlin.de/people/mielke/

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