Ergodicity in bidimensional sphere systems

In the framework of Piecewise Deterministic Markov Processes

Athina Monemvassitis

Online workshop on ECMC and related subjects

May 11, 2021

Collaborators : A. Guillin, M. Michel, S. Monteil
Laboratoire de Mathémathiques Blaise Pascal - Université Clermont Auvergne
athina.monemvassitis@uca.fr

Markov Chain - discrete time

Markov chain on Ω, $\{X_n;\ n \in \mathbb{N}_N\}$

$$\forall n \in \mathbb{N}_N,\ X_n \sim \pi \implies \frac{1}{N}\sum_{n=0}^{N} f(X_n) \underset{N \to +\infty}{\longrightarrow} \sum_{x \in \Omega} f(x)\pi(x)$$

- Global balance condition

$$\int_\Omega \pi(x')P_{x'x}\mathrm{d}x' = \int_\Omega \pi(x)P_{xx'}\mathrm{d}x'$$

- Detailed balance condition

$$\forall (x, x') \in \Omega,\ \pi(x')P_{x'x} = \pi(x)P_{xx'}$$

Markov Chain - discrete time

Markov chain on Ω, $\{X_n;\, n \in \mathbb{N}_N\}$

$$\forall n \in \mathbb{N}_N,\, X_n \sim \pi \implies \frac{1}{N}\sum_{n=0}^{N} f(X_n) \underset{N\to+\infty}{\longrightarrow} \sum_{x\in\Omega} f(x)\pi(x)$$

- Global balance condition

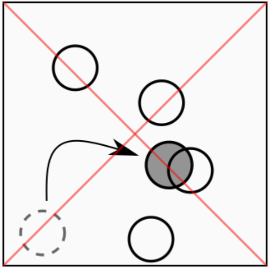
$$\int_\Omega \pi(x')P_{x'x}\mathrm{d}x' = \int_\Omega \pi(x)P_{xx'}\mathrm{d}x'$$

- Detailed balance condition

$$\forall (x,x') \in \Omega,\, \pi(x')P_{x'x} = \pi(x)P_{xx'}$$

Metropolis algorithm $P_{x_i x_i'} = a(x_i'|x_i)p^{\mathrm{acc}}(x_i \to x_i')$,

$$p^{\mathrm{acc}}(x_i \to x_i') = \exp(-\beta[\sum_{j\neq i} \Delta E(x_i', x_j)])^{+}$$



Markov Chain - discrete time

Markov chain on Ω, $\{X_n;\ n \in \mathbb{N}_N\}$

$$\forall n \in \mathbb{N}_N,\ X_n \sim \pi \implies \frac{1}{N}\sum_{n=0}^{N} f(X_n) \underset{N\to+\infty}{\longrightarrow} \sum_{x\in\Omega} f(x)\pi(x)$$

- Global balance condition

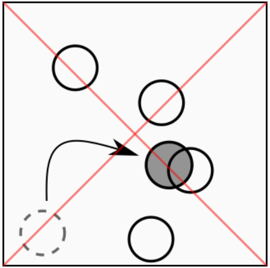
$$\pi P = \pi$$

- Detailed balance condition

$$\forall (x, x') \in \Omega,\ \pi(x')P_{x'x} = \pi(x)P_{xx'}$$

Metropolis algorithm $P_{x_i x_i'} = a(x_i'|x_i)p^{\mathrm{acc}}(x_i \to x_i')$,

$$p^{\mathrm{acc}}(x_i \to x_i') = \exp(-\beta[\sum_{j\neq i} \Delta E(x_i', x_j)])^+$$



Markov Chain - continuous time

Markov chain on $\Omega \times V$, $\{X_n;\ n \in \mathbb{N}_N\}$

$$\forall n \in \mathbb{N}_N,\ X_n \sim \pi \implies \frac{1}{N}\sum_{n=0}^{N} f(X_n) \underset{N\to+\infty}{\longrightarrow} \sum_{x\in\Omega} f(x)\pi(x)$$

- Global balance condition

$$\pi P = \pi$$

- Break Detailed balance condition : Event-Chain algorithms
  - Extension of the space $\Omega \to \Omega \times V$

Markov Chain - continuous time

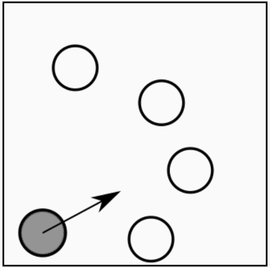
Markov chain on $\Omega \times V$, $\{X_n;\, n \in \mathbb{N}_N\}$

$$\forall n \in \mathbb{N}_N,\ X_n \sim \pi \implies \frac{1}{N}\sum_{n=0}^{N} f(X_n) \xrightarrow[N\to+\infty]{} \sum_{x\in\Omega} f(x)\pi(x)$$

- Global balance condition

$$\pi P = \pi$$

- Break Detailed balance condition : Event-Chain algorithms
  - Extension of the space $\Omega \to \Omega \times V$
    Lifting framework $x \to (x, v)$, $\pi \to \pi \otimes \mu_V$



Markov Chain - continuous time

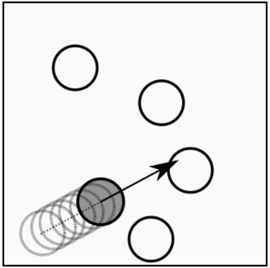
Markov chain on $\Omega \times V$, $\{X_n;\ n \in \mathbb{N}_N\}$

$$\forall n \in \mathbb{N}_N,\ X_n \sim \pi \implies \frac{1}{N}\sum_{n=0}^{N} f(X_n) \underset{N\to+\infty}{\longrightarrow} \sum_{x\in\Omega} f(x)\pi(x)$$

- Global balance condition

$$\pi P = \pi$$

- Break Detailed balance condition : Event-Chain algorithms
  - Extension of the space $\Omega \to \Omega \times V$
    Lifting framework $x \to (x, v)$, $\pi \to \pi \otimes \mu_V$
  - Continuous time
    $p^{\mathrm{acc}}_{\mathrm{fac}}(x \to x' = x + T \cdot v) = \exp(-\beta \int_0^T [\nabla_x E(x + s \cdot v) \cdot v]^+ \mathrm{d}s)$



Markov Chain - continuous time

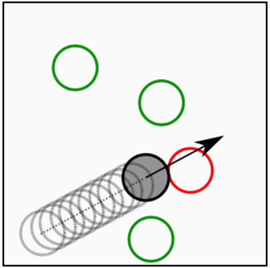
Markov chain on $\Omega \times V$, $\{X_n;\ n \in \mathbb{N}_N\}$

$$\forall n \in \mathbb{N}_N,\ X_n \sim \pi \implies \frac{1}{N}\sum_{n=0}^{N} f(X_n) \underset{N\to+\infty}{\longrightarrow} \sum_{x\in\Omega} f(x)\pi(x)$$

- Global balance condition

$$\pi P = \pi$$

- Break Detailed balance condition : Event-Chain algorithms
  - Extension of the space $\Omega \to \Omega \times V$
    Lifting framework $x \to (x, v)$, $\pi \to \pi \otimes \mu_V$
  - Continuous time
    $p^{\mathrm{acc}}_{\mathrm{fac}}(x \to x' = x + T \cdot v) = \exp(-\beta \int_0^T [\nabla_x E(x + s\cdot v)\cdot v]^+ \mathrm{d}s)$
  - Factorization
    $p^{\mathrm{acc}}_{\mathrm{fac}}(x_i \to x_i') = \exp(-\beta \sum_{j\neq i} \int_0^{T_i} [\nabla_{x_i} E(x_i + s\cdot v, x_j)\cdot v]^+ \mathrm{d}s)$



Markov Chain - continuous time

- New dynamics : Event-chain algorithms
  - Physical moves
    $(x, v = (e, i)) \to (x', v) = (x + t_i^* e, v)$
  - Lifting moves
    $(x, v = (e, i)) \to (x, v' = (e', i'))$

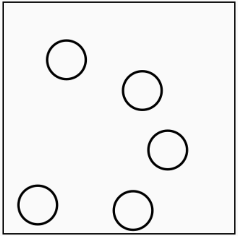
  - Change of direction

    At a lifting event, $v' \sim \rho((x, v), (x, v'))$
    where $\rho((x, v), (x, v')) = \delta(e - e')\delta(i - i')$

    At a refreshment, $v' \sim \mu_V(v)$

  - Events drawn from Poisson processes of rates

$$\int_0^{t_{ij}} [\nabla_{x_i} E(x_i + s \cdot v, x_j) \cdot v]^+ \mathrm{d}s$$



Markov Chain - continuous time

- New dynamics : Event-chain algorithms
  - Physical moves
    $(x, v = (e, i)) \to (x', v) = (x + t_i^* e, v)$
  - Lifting moves
    $(x, v = (e, i)) \to (x, v' = (e', i'))$

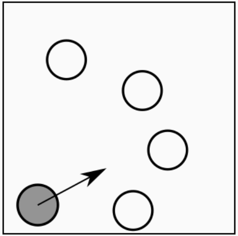
  - Change of direction

    At a lifting event, $v' \sim \rho((x, v), (x, v'))$
    where $\rho((x, v), (x, v')) = \delta(e - e')\delta(i - i')$

    At a refreshment, $v' \sim \mu_V(v)$

  - Events drawn from Poisson processes of rates

$$\int_0^{t_{ij}} [\nabla_{x_i} E(x_i + s \cdot v, x_j) \cdot v]^+ \mathrm{d}s$$



Markov Chain - continuous time

- New dynamics : Event-chain algorithms
  - Physical moves
    $(x, v = (e, i)) \to (x', v) = (x + t_i^* e, v)$
  - Lifting moves
    $(x, v = (e, i)) \to (x, v' = (e', i'))$

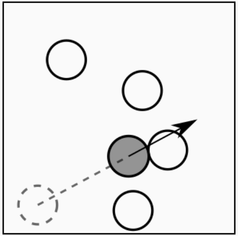
  - Change of direction

    At a lifting event, $v' \sim \rho((x, v), (x, v'))$
    where $\rho((x, v), (x, v')) = \delta(e - e')\delta(i - i')$

    At a refreshment, $v' \sim \mu_V(v)$

  - Events drawn from Poisson processes of rates

$$\int_0^{t_{ij}} [\nabla_{x_i} E(x_i + s \cdot v, x_j) \cdot v]^+ \mathrm{d}s$$



Markov Chain - continuous time

- New dynamics : Event-chain algorithms
    - Physical moves
      $(x, v = (e, i)) \to (x', v) = (x + t_i^* e, v)$
    - Lifting moves
      $(x, v = (e, i)) \to (x, v' = (e', i'))$

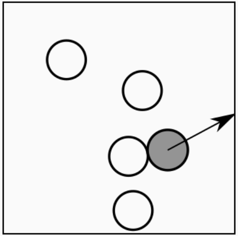
    - Change of direction

      At a lifting event, $v' \sim \rho((x, v), (x, v'))$
      where $\rho((x, v), (x, v')) = \delta(e - e')\delta(i - i')$

      At a refreshment, $v' \sim \mu_V(v)$

    - Events drawn from Poisson processes of rates

$$\int_0^{t_{ij}} [\nabla_{x_i} E(x_i + s \cdot v, x_j) \cdot v]^+ \mathrm{d}s$$



Markov Chain - continuous time

- New dynamics : Event-chain algorithms
  - Physical moves
    $(x, v = (e, i)) \to (x', v) = (x + t_i^* e, v)$
  - Lifting moves
    $(x, v = (e, i)) \to (x, v' = (e', i'))$

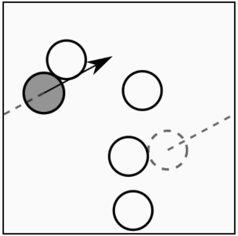
  - Change of direction

    At a lifting event, $v' \sim \rho((x, v), (x, v'))$
    where $\rho((x, v), (x, v')) = \delta(e - e')\delta(i - i')$

    At a refreshment, $v' \sim \mu_V(v)$

  - Events drawn from Poisson processes of rates

$$\int_0^{t_{ij}} [\nabla_{x_i} E(x_i + s \cdot v, x_j) \cdot v]^+ \mathrm{d}s$$



Markov Chain - continuous time

- New dynamics : Event-chain algorithms
  - Physical moves
    $(x, v = (e, i)) \to (x', v) = (x + t_i^* e, v)$
  - Lifting moves
    $(x, v = (e, i)) \to (x, v' = (e', i'))$

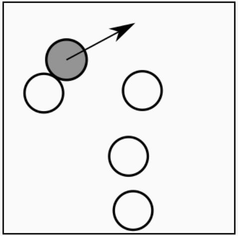
  - Change of direction

    At a lifting event, $v' \sim \rho((x, v), (x, v'))$
    where $\rho((x, v), (x, v')) = \delta(e - e')\delta(i - i')$

    At a refreshment, $v' \sim \mu_V(v)$

  - Events drawn from Poisson processes of rates

$$\int_0^{t_{ij}} [\nabla_{x_i} E(x_i + s \cdot v, x_j) \cdot v]^+ \mathrm{d}s$$



Markov Chain - continuous time

- New dynamics : Event-chain algorithms
  - Physical moves
    $(x, v = (e, i)) \to (x', v) = (x + t_i^* e, v)$
  - Lifting moves
    $(x, v = (e, i)) \to (x, v' = (e', i'))$

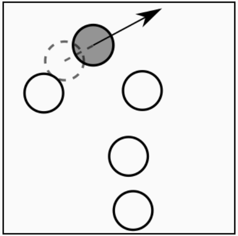
  - Change of direction

    At a lifting event, $v' \sim \rho((x, v), (x, v'))$
    where $\rho((x, v), (x, v')) = \delta(e - e')\delta(i - i')$

    At a refreshment, $v' \sim \mu_V(v)$

  - Events drawn from Poisson processes of rates

$$\int_0^{t_{ij}} [\nabla_{x_i} E(x_i + s \cdot v, x_j) \cdot v]^+ \mathrm{d}s$$



Markov Chain - continuous time

- New dynamics : Event-chain algorithms
  - Physical moves
    $(x, v = (e, i)) \to (x', v) = (x + t_i^* e, v)$
  - Lifting moves
    $(x, v = (e, i)) \to (x, v' = (e', i'))$

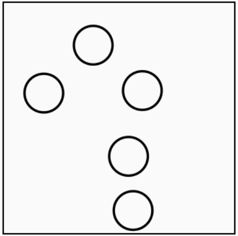
  - Change of direction

    At a lifting event, $v' \sim \rho((x, v), (x, v'))$
    where $\rho((x, v), (x, v')) = \delta(e - e')\delta(i - i')$

    At a refreshment, $v' \sim \mu_V(v)$

  - Events drawn from Poisson processes of rates

$$\int_0^{t_{ij}} [\nabla_{x_i} E(x_i + s \cdot v, x_j) \cdot v]^+ \mathrm{d}s$$



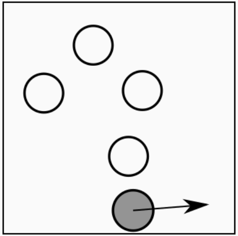
Markov Chain - continuous time

- New dynamics : Event-chain algorithms
  - Physical moves
    $(x, v = (e, i)) \to (x', v) = (x + t_i^* e, v)$
  - Lifting moves
    $(x, v = (e, i)) \to (x, v' = (e', i'))$
  - Change of direction

    At a lifting event, $v' \sim \rho((x, v), (x, v'))$
    where $\rho((x, v), (x, v')) = \delta(e - e')\delta(i - i')$

    At a refreshment, $v' \sim \mu_V(v)$
  - Events drawn from Poisson processes of rates

$$\int_0^{t_{ij}} [\nabla_{x_i} E(x_i + s \cdot v, x_j) \cdot v]^+ \mathrm{d}s$$



Markov Chain - continuous time

- New dynamics : Event-chain algorithms
  - Physical moves
    $(x, v = (e, i)) \to (x', v) = (x + t_i^* e, v)$
  - Lifting moves
    $(x, v = (e, i)) \to (x, v' = (e', i'))$
  - Change of direction
    At a lifting event, $v' \sim \rho((x, v), (x, v'))$
    where $\rho((x, v), (x, v')) = \delta(e - e')\delta(i - i')$

    At a refreshment, $v' \sim \mu_V(v)$
  - Events drawn from Poisson processes of rates

$$\int_0^{t_{ij}} [\nabla_{x_i} E(x_i + s \cdot v, x_j) \cdot v]^+ \mathrm{d}s$$

- Piecewise deterministic Markov process
  - Deterministic flow
    $\phi_t(x, v = (e, i)) = (x + te, v)$
  - Markov kernels $\{Q_k((x, v), \mathrm{d}\tilde{v})\}$
    $Q_k((x, v), \mathrm{d}\tilde{v}) = \delta(e - \tilde{e})\delta(i - \tilde{i})\mathrm{d}\tilde{e}\mathrm{d}\tilde{i}$
  - Jump rate $\lambda^{\mathrm{tot}} = \sum_k \lambda_k + \lambda_r$
    $\lambda_k(x, v = (e, i)) = [\nabla_{x_i} E(x_i, x_k) \cdot e]^+$

    Refreshment rate $\lambda_r \in \mathbb{R}_+^*$
  - Events drawn from Poisson processes of rates

$$\int_0^{t_{ik}} \lambda_k(\phi_s(x, v), v)\mathrm{d}s$$

Piecewise Deterministic Markov Process (PDMP)

General formulation

The PDMP (X_t, V_t) defined on $\Omega \times V$ is characterized by

- A deterministic flow $(\phi_t)_{t\geq 0}$,
- A Markov kernel $Q((x,v),\mathrm{d}\tilde{v}) = \delta(v-\tilde{v})\mathrm{d}v$
- A jump rate $\lambda^{\mathrm{tot}} = \lambda + \lambda_r$, $\lambda(x,v) = [\nabla_x E(x)\cdot v]^+$, $\lambda_r \in \mathbb{R}_+^*$

and targets the extended probability distribution $\bar{\pi} = \pi \otimes \mu_V$.

It defines a Markov semi-group $(P_t)_{t\geq 0}$, writing for $A \in \mathcal{B}(\Omega \times V)$

$$P_t((x,v),A) = \mathbb{P}((X_t, V_t) \in A).$$

The infinitesimal generator, encoding infinitesimal changes in $(P_t)_{t\geq 0}$ is defined as

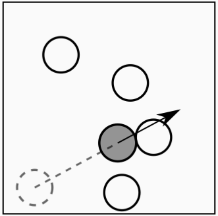
$$\mathcal{A}f = \lim_{t\to 0^+} \frac{P_t f - f}{t},$$

Piecewise Deterministic Markov Process (PDMP) - Invariance

The infinitesimal generator reads

$$\mathcal{A}f(x,v) = \underbrace{\nabla_x f(x,v)\cdot v}_{\text{transport}} + \underbrace{[\nabla_x E(x)\cdot v]_+ \left(\int_V f(x,\tilde{v})Q((x,v),\mathrm{d}\tilde{v}) - f(x,v)\right)}_{\text{event}}$$

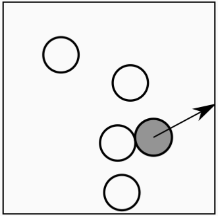
$$+ \underbrace{\lambda_r \left(\int_V f(x,\tilde{v})\mathrm{d}\mu_V(\tilde{v}) - f(x,v)\right)}_{\text{refreshment}}$$



Piecewise Deterministic Markov Process (PDMP) - Invariance

The infinitesimal generator reads

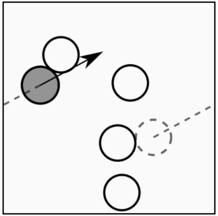
$$\mathcal{A}f(x,v) = \underbrace{\nabla_x f(x,v)\cdot v}_{\text{transport}} + \underbrace{[\nabla_x E(x)\cdot v]_+ \left(\int_V f(x,\tilde v) Q((x,v),\mathrm{d}\tilde v) - f(x,v)\right)}_{\text{event}}$$
$$+ \underbrace{\lambda_r \left(\int_V f(x,\tilde v)\mathrm{d}\mu_V(\tilde v) - f(x,v)\right)}_{\text{refreshment}}$$



Piecewise Deterministic Markov Process (PDMP) - Invariance

The infinitesimal generator reads

$$\mathcal{A}f(x,v) = \underbrace{\nabla_x f(x,v)\cdot v}_{\text{transport}} + \underbrace{[\nabla_x E(x)\cdot v]_+ \left(\int_V f(x,\tilde{v})Q((x,v),\mathrm{d}\tilde{v}) - f(x,v)\right)}_{\text{event}}$$
$$+ \underbrace{\lambda_r \left(\int_V f(x,\tilde{v})\mathrm{d}\mu_V(\tilde{v}) - f(x,v)\right)}_{\text{refreshment}}$$

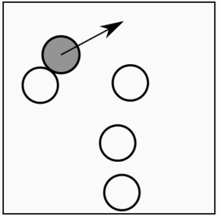


Piecewise Deterministic Markov Process (PDMP) - Invariance

The infinitesimal generator reads

$$\mathcal{A}f(x,v) = \underbrace{\nabla_x f(x,v)\cdot v}_{\text{transport}} + \underbrace{[\nabla_x E(x)\cdot v]_+ \left(\int_V f(x,\tilde v) Q((x,v),\mathrm{d}\tilde v) - f(x,v)\right)}_{\text{event}}$$

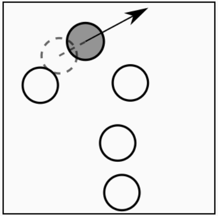
$$+ \underbrace{\lambda_r \left(\int_V f(x,\tilde v)\mathrm{d}\mu_V(\tilde v) - f(x,v)\right)}_{\text{refreshment}}$$



Piecewise Deterministic Markov Process (PDMP) - Invariance

The infinitesimal generator reads

$$\mathcal{A}f(x,v) = \underbrace{\nabla_x f(x,v)\cdot v}_{\text{transport}} + \underbrace{[\nabla_x E(x)\cdot v]_+ \left(\int_V f(x,\tilde v) Q((x,v),\mathrm{d}\tilde v) - f(x,v)\right)}_{\text{event}}$$
$$+ \underbrace{\lambda_r \left(\int_V f(x,\tilde v)\mathrm{d}\mu_V(\tilde v) - f(x,v)\right)}_{\text{refreshment}}$$

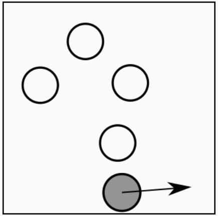


Piecewise Deterministic Markov Process (PDMP) - Invariance

The infinitesimal generator reads

$$\mathcal{A}f(x,v) = \underbrace{\nabla_x f(x,v)\cdot v}_{\text{transport}} + \underbrace{[\nabla_x E(x)\cdot v]_+ \left(\int_V f(x,\tilde{v}) Q((x,v),\mathrm{d}\tilde{v}) - f(x,v)\right)}_{\text{event}}$$

$$+ \underbrace{\lambda_r \left(\int_V f(x,\tilde{v})\mathrm{d}\mu_V(\tilde{v}) - f(x,v)\right)}_{\text{refreshment}}$$



Piecewise Deterministic Markov Process (PDMP) - Invariance

The infinitesimal generator reads

$$\mathcal{A}f(x,v) = \underbrace{\nabla_x f(x,v)\cdot v}_{\text{transport}} + \underbrace{[\nabla_x E(x)\cdot v]_+ \left(\int_V f(x,\tilde{v})Q((x,v),\mathrm{d}\tilde{v}) - f(x,v)\right)}_{\text{event}}$$
$$+ \underbrace{\lambda_r \left(\int_V f(x,\tilde{v})\mathrm{d}\mu_V(\tilde{v}) - f(x,v)\right)}_{\text{refreshment}}$$

and with $\bar{\pi} = \pi \otimes \mu_V$, if $\bar{\pi}P_t = \bar{\pi}$,

$$\int_{\Omega\times V} \mathcal{A}f\,\mathrm{d}\bar{\pi} = 0 \qquad \text{(Invariance)}$$

Uniform ergodicity

For any $(x_0, v_0) \in \Omega \times V$ and $A \in \mathcal{B}(\Omega \times V)$,

$$\int \mathbb{P}_{(\mathbf{x_0},\mathbf{v_0})}((X_t, V_t) \in A) \geq c\nu(A) \qquad \text{(Petite set)}$$

where $c \in \mathbb{R}_+^*$ and ν a non-trivial measure.

- Difficulties
  - $\int \mathbb{P}_{(\mathbf{x_0},\mathbf{v_0})}((X_t, V_t) \in A) \propto d(x_{t,i}, x_{t,j})$ for all $t \geq 0$
  - Metropolis algorithm : density obtained at each step
    ECMC / PDMP : uses only events and refreshments to create density
- Solutions
  - Control of distances for all intermediate sets of configurations
  - Create a density of paths conecting any two states through refreshments

Connectivity in bidimensional hard sphere systems

Connectivity of Ω_H : there is a path connecting any two points in Ω_H

With $\Omega_H = \{x \in \Omega, \forall (i,j) \in [\![1,N]\!]^2, d(x_i,x_j) > 2\sigma\}$, and $\sqrt{N}\sigma < \alpha_0$,

$$\int \mathbb{P}_{(x_0,v_0)}((X_t,V_t) \in A) > 0$$

which improves on Diaconis, P., Lebeau, G., & Michel, L. (2011).

- Difficulties
  - Too strict condition on the density to apply the same scheme as the previous proof
  - Critical density for connectivity is still an open question
- Scheme of proof
  - Expansion of a configuration to ensure a minimal distance between each pair of spheres
  - Connectivity of the set of expanded configurations
  - Existence of paths connecting the expanded and the contracted sets

Conclusion

- ECMC algorithms can be cast in the framework of PDMP
- Efficient tool to explore invariance and ergodicity of stochastic processes

- Proof for invariance and ergodicity in bidimensional soft sphere systems
- Proof for invariance and connectivity in bidimensional soft sphere systems

Conclusion

- ECMC algorithms can be cast in the framework of PDMP
- Efficient tool to explore invariance and ergodicity of stochastic processes

- Proof for invariance and ergodicity in bidimensional soft sphere systems
- Proof for invariance and connectivity in bidimensional soft sphere systems

Thank you for your attention !