Non-reversible sampling of hardcore particle systems

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Analysis and simulations of metastable systems Conference, CIRM, Marseille

Joint work with Arnaud Guillin, Tristan Guyon and Athina Monemvassitis (UCA)

Outline

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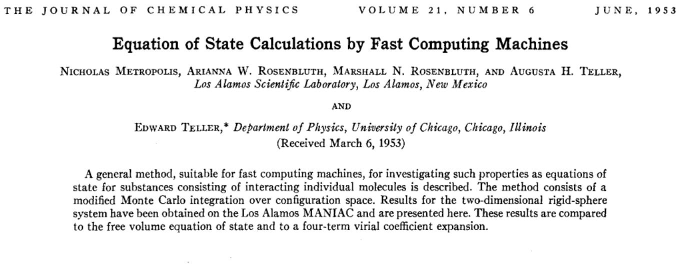
THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

Equation of State Calculations by Fast Computing Machines

Nicholas Metropolis, Arianna W. Rosenbluth, Marshall N. Rosenbluth, and Augusta H. Teller,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

and

Edward Teller,* *Department of Physics, University of Chicago, Chicago, Illinois*
(Received March 6, 1953)

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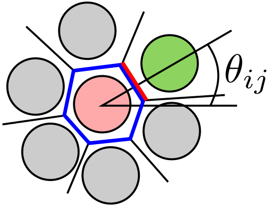
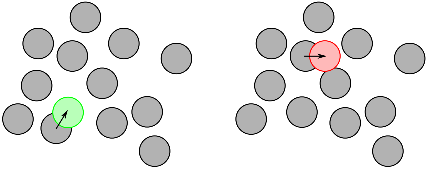


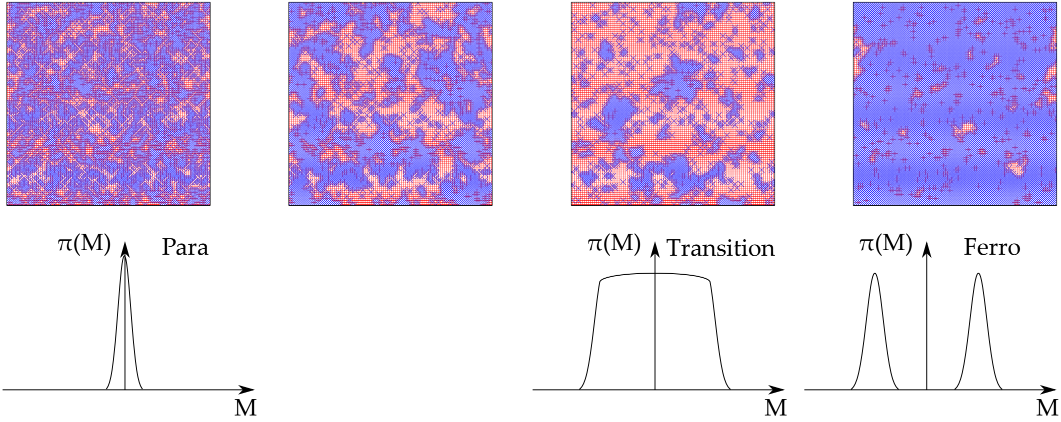
Metropolis algorithm



Diffusive dynamics

- Correlated sample: $\sigma^2(\bar{\Theta}) \propto \tau(\Theta)$
  $C_\Theta(t) = \frac{\langle \Theta(t'+t)\Theta(t')\rangle - \langle \Theta^2 \rangle}{\langle \Theta^2 \rangle - \langle \Theta \rangle^2}$
- Around 2nd order phase transition $\tau \propto \xi^z \propto L^z$
  $C_\Theta(t) \sim \exp(-t/\tau)$

Cluster algorithms (Swendsen and Wang (1987), Wolff (1989))



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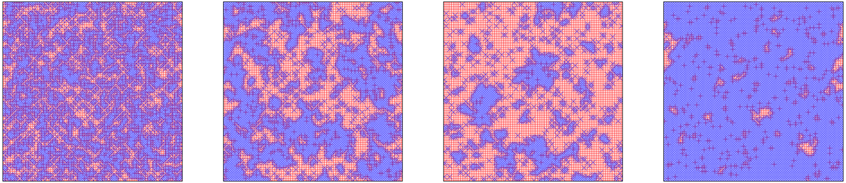
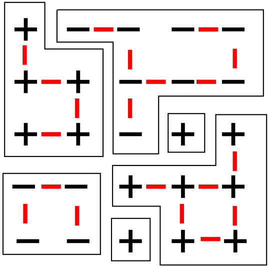


Cluster algorithms (Swendsen-Wang et al (1987); Wolff et al (1989))



- Instead of single-spin flip, flip of correlated-spin clusters $\rightarrow$ reduction of critical slowing down
- Create or not a bond between neighboring spins.
- Pick a random value for each newly built cluster

Detailed balance is fulfilled: flipping is involutary

$q(x', x)/q(x, x') = \pi(x')/\pi(x) =$ no rejection

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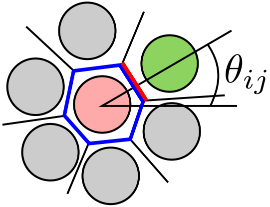
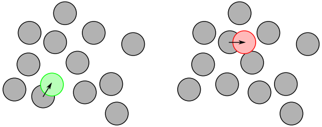
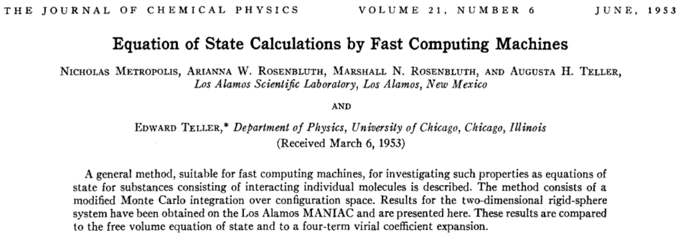


Metropolis algorithm



How to produce collective moves?

- Continuous state space. No discrete symmetry as for spin lattices to easily build global q.
- With detailed balance in hard-core particle systems: symmetric proposal probabilities are necessary for the scheme to be rejection-free.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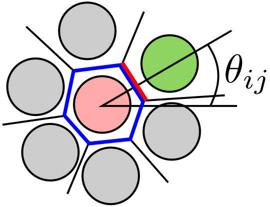

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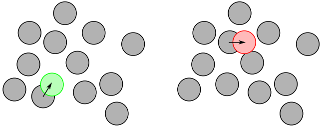

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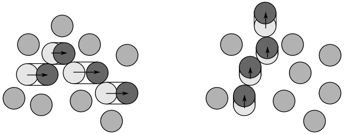
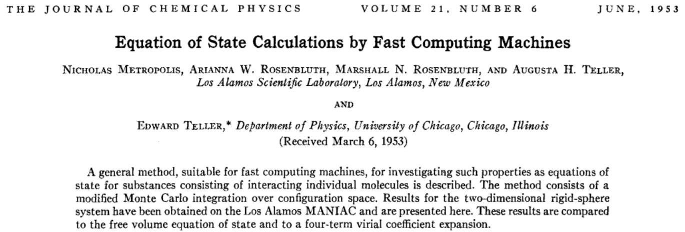
- Break DB: Non-reversibility?





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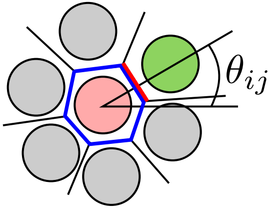
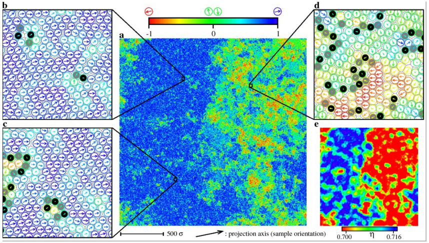
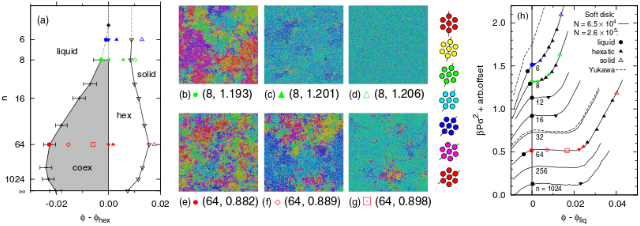


Event-chain Monte Carlo

Bernard et al (2009)

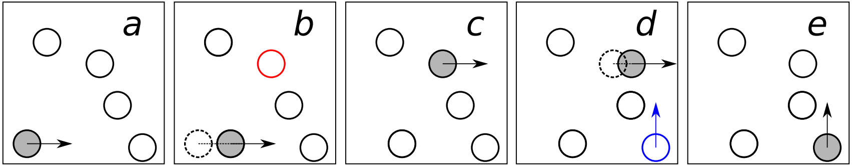


Michel et al (2014), Kapfer et al (2015)



Outline

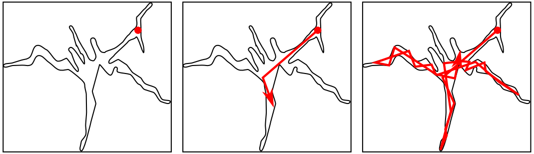
Event-chain Monte Carlo



- (a) A sphere is updated ballistically.
- (b-c) At some point, an *event* with another sphere is triggered and the ballistic flow is updated.
  $a_{\text{Met}} = \exp(-[\sum_j \delta E_{ij}]_+) \to a_{\text{Fact}} = \exp(-\sum_j [\delta E_{ij}]_+) \underset{\delta\to 0}{\to} 1 - \beta \sum_j [\mathrm{d}E_{ij}]_+$
- (d-e) A *refreshment* is triggered and the ballistic flow is updated.

ECMC is rejection-free and relies on a control by the events of the ballistic exploration to ensure the correct invariant distribution.

Piecewise Deterministic Markov Process



PDMP characterizing elements (Davis (1993), in MCMC: Bouchard-Côté et al (2018), Bierkens et al (2018))

- Differential flow $(\phi_t)_{t\geq 0}$
- Jump rate $\lambda(x, e) + \bar{\lambda}$
- Markov kernel Q

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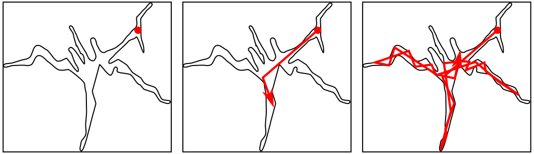

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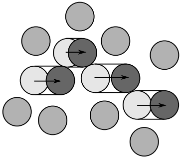
Infinitesimal generator $\mathcal{A}f=\lim_{t\to 0}\frac{P_t f - f}{t}$, $D_\phi f(x,e)=\lim_{t\to 0}\frac{f(\phi_t(x,e))-f(x,e)}{t}$

$$\mathcal{A}f=\underbrace{D_\phi f(x,e)}_{\text{Transport}}+\underbrace{\lambda(x,e)\int_{\mathcal{V}}(f(x,e')-f(x,e))Q((x,e),\mathrm{d}e')}_{\text{Events - Direction changes}}+\underbrace{\bar{\lambda}\int_{\mathcal{V}}(f(x,e')-f(x,e))\mu(\mathrm{d}e')}_{\text{Refreshment}}$$

ECMC in isotropic particle systems



- Particle systems, $E(x) = \sum_{i,j} E_{ij}(x)$,
  $v = (e, i) \in \{(0,1), (1,0)\} \times \{1..N\}$

Michel et al (2014), Monemvassitis et al (2023)

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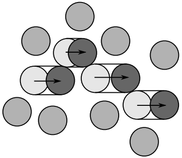

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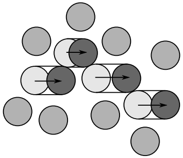

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- Event rate $\sum_j \lambda_j(x, (e, i)) = \sum_j \langle \boldsymbol{\nabla}_{x_i} E_{ij}(x), e \rangle_+$
- Markov kernel $Q_j((x, (e, i)), \mathrm{d}i'\mathrm{d}e') = \delta(j - i')\delta(e - e')\mathrm{d}e'\mathrm{d}i'$

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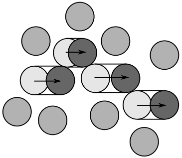

Soft spheres

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$$\mathcal{A}f(x,(e,i)) = \langle \nabla_{x_i} f(x,(e,i)) + \sum_{k=1}^{N} \lambda_k(x,(e,i)) \left(\int_{\mathcal{V}} Q_k((x,(e,i)), \mathrm{d}e', \mathrm{d}i') f(x,(e',i')) - f(x,(e,i)) \right)$$

Michel et al (2014), Monemvassitis et al (2023)

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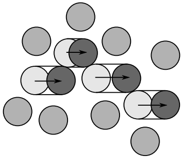

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Hard spheres = boundary effect

$$\begin{cases} \mathcal{A}f(x,(e,i)) = & \langle \nabla_{x_i} f(x,(e,i)), e\rangle, e\rangle, (x,(e,i) \in E \\ Q^b((x,(e,i)), A) = & \sum_{k=1,\neq i}^{N} \int_{\mathcal{V}} \mathbb{1}_A(x,(e',i')) Q_k(x,(e,i), \mathrm{d}e', \mathrm{d}i'), (x,(e,i)) \in \partial E \end{cases}$$

Michel et al (2014), Monemvassitis et al (2023)

Refreshment at fixed time = a boundary effect

Common: exponential refreshment

$(x, v) \in E = \Omega \times \mathcal{V}$

$$\begin{cases} \mathcal{A}f(x,v) = & \langle \nabla_x f(x,v), v \rangle + \lambda(x,v) \left(\int_{\mathcal{V}} Q((x,v), \mathrm{d}v') f(x,v') - f(x,v) \right) \\ & + \lambda_r \left(\int_{\mathcal{V}} f(x,v') \mathrm{d}\mu_{\mathcal{V}}(v') - f(x,v) \right), (x,v) \in E \\ Q^b((x,v),A) = & \int_{\mathcal{V}} \mathbb{1}_A(x,v') K(v, \mathrm{d}v'), (x,v) \in \partial E \end{cases}$$

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$\rightarrow$ Describe it as a boundary effect, $l \in \mathcal{L}$, $\partial\mathcal{L} = 0$, $(x, v, l) \in E = \Omega \times \mathcal{V} \times \mathcal{L}$

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Monemvassitis et al (2023)

Refreshment as a boundary effect

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Conditions on R and μ_L: Transport by $-\partial_l$ compensated by R-jump

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\mu_L(0^+) R(0,\mathrm{d}l) = (-\partial_l \mu_L(l))\mathrm{d}l \iff \mu_L(l) = h(l)\mathbb{1}_L,
$$

where $L \subset \mathcal{L}$ and h decreasing over L so that $h(0^+) > 0$, $\int_{\mathcal{L}} \frac{-\partial_l \mu_L(l)}{\mu_L(0^+)}\mathrm{d}l = 1$

Monemvassitis et al (2023)

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Refreshment as a boundary effect

Conditions on R and μ_L: Transport by $-\partial_l$ compensated by R-jump

$$\mu_L(0^+)R(0, \mathrm{d}l) = (-\partial_l \mu_L(l))\mathrm{d}l \iff \mu_L(l) = h(l)\mathbb{1}_L,$$

where $L \subset \mathcal{L}$ and h decreasing over L so that $h(0^+) > 0$, $\int_{\mathcal{L}} \frac{-\partial_l \mu_L(l)}{\mu_L(0^+)}\mathrm{d}l = 1$

Recovering exponential and fixed-time refreshment

$$\begin{cases} \text{fixed-time } T\text{: } \mu_L(l) = \frac{1}{T}\mathbb{1}_{]0,T[}\text{and } R(l, \mathrm{d}l') = \delta(l' - T)\mathrm{d}l', \text{ with } T > 0, L =]0, T] \\ \text{exponential of rate } \lambda_r\text{: } \mu_L(l) = \lambda_r e^{-\lambda_r l}\mathbb{1}_{l>0}\text{and } R(l, \mathrm{d}l') = \lambda_r e^{-\lambda_r l'}\mathbb{1}_{l'>0}\mathrm{d}l', \text{ with } \lambda_r > 0, L = \mathcal{L} \end{cases}$$

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But also

- $\mu_L(l) = A(T-l)^k\mathbb{1}_{0<l\leq T}$, and refreshment $R(0,\mathrm{d}l) = \frac{k}{T^k}(T-l)^{k-1}\mathbb{1}_{0<l\leq T}$,
- $\mu_L(l) = \frac{A}{(T+l)^k}\mathbb{1}_{0<l}$, and refreshment $R(0,\mathrm{d}l) = \frac{kT^k}{(T+l)^{k+1}}\mathbb{1}_{0<l}$,
- $\mu_L(l) = Ae^{-Tl^k}\mathbb{1}_{0<l}$, and refreshment $R(0,\mathrm{d}l) = kTl^{k-1}e^{-Tl^k}\mathbb{1}_{0<l}$, etc

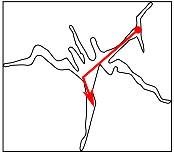
where $(T,k) \in \mathbb{R}_+^{*2}$, $l \in \mathcal{L}$ and A is a suitable normalization constant. Monemvassitis et al (2023)

Invariance: Transport compensated by the direction changes

Infinitesimal generator $\mathcal{A}f = \lim_{t\to 0} \frac{P_t f - f}{t}$

$$\mathcal{A}f = \underbrace{D_\phi f(x,e)}_{\text{Transport}} + \underbrace{\lambda(x,e)\int_{\mathcal{V}}(f(x,e') - f(x,e))Q((x,e),\mathrm{d}e')}_{\text{Events - Direction changes}} + \underbrace{\bar{\lambda}\int_{\mathcal{V}}(f(x,e') - f(x,e))\mu(\mathrm{d}e')}_{\text{Refreshment}}$$

Conditions for $\tilde{\pi} = \pi \times \mu$ invariant: $\int_{\Omega\times\mathcal{V}} \mathcal{A}f \,\mathrm{d}\pi\mathrm{d}\mu = 0$



$$\int_{\Omega\times\mathcal{V}} D_\phi f(x,e)\pi(\mathrm{d}x)\mu(\mathrm{d}e)$$
$$= \int_{\Omega\times\mathcal{V}}\int_{\mathcal{V}} \lambda(x,e)(f(x,e') - f(x,e))Q((x,e),\mathrm{d}e')\pi(\mathrm{d}x)\mu(\mathrm{d}e)$$

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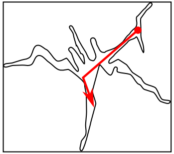

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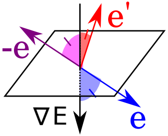
With a flow along e, by integration by part, $(\pi(x) \propto \exp(-E(x)))$

$$\underbrace{\int_{\mathcal{V}} \langle \nabla E(x), -e'\rangle_+ f(x,e')\mu(\mathrm{d}e')}_{\text{brought by transport}} = \underbrace{\int_{\mathcal{V}}\int_{\mathcal{V}} \langle \nabla E(x), e\rangle_+ f(x,e') Q((x,e),\mathrm{d}e')\mu(\mathrm{d}e)}_{\text{redistribution by direction change}}$$



Designing events through global symmetry exploitation

$$\underbrace{\int_{\mathcal{V}} \langle \nabla E(x), -e' \rangle_+ f(x,e') \mu(\mathrm{d}e')}_{\text{brought by transport}} = \underbrace{\int_{\mathcal{V}} \int_{\mathcal{V}} \langle \nabla E(x), e' \rangle_+ f(x,e) Q((x,e'),\mathrm{d}e) \mu(\mathrm{d}e')}_{\text{redistribution by direction change}}$$

- Exploitation of mirror symmetry through factorization (Michel et al 2014)

$$\nabla_{x_i} E_{ij}(x) = -\nabla_{x_j} E_{ij}(x) \text{ (i.e. } \mathrm{div} E_{ij} = 0) \rightarrow Q_j((x,(e,i)),\mathrm{d}i'\mathrm{d}e') = \delta(j-i')\delta(e-e')\mathrm{d}e'\mathrm{d}i'$$

$$\rightarrow Q_j((x,(e,i)),\mathrm{d}i'\mathrm{d}e') = \delta(j-i')\delta(e-R_x(e'))\mathrm{d}e'\mathrm{d}i'$$

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- Exploitation of translational invariance (Harland et al 2017)

$$\nabla \cdot E = 0 \to Q((x,(e,i)),\mathrm{d}i'\mathrm{d}e') = \sum_k \frac{\langle \nabla_{x_k} E, e \rangle_-}{\sum_j \langle \nabla_{x_j} E, e \rangle_+} \delta(e-e')\delta(k-i')\mathrm{d}e'\mathrm{d}i'$$

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- Exploitation of rotational invariance (Michel et al 2020)

$$\int \langle \nabla E, e \rangle \mu(\mathrm{d}e) = 0 \to Q((x,(e,i)),\mathrm{d}i'\mathrm{d}e') \propto \langle \nabla E, e' \rangle_- \mu(\mathrm{d}e')(\ldots \mathrm{d}i')$$

Outline

Pitfalls of hardcore particle sampling

Non-reversible and continuous-time sampling by ECMC

Invariance through interplay of transport and direction changes

Ergodicity

Generalized deterministic flow

Anisotropic hardcore particles

Ergodicity in sphere systems

Ergodicity in PDMP

- Goal is to find a density of paths connecting two states, while probability minorization (positive Harris recurrent, irreducible skeleton chain, Meyn and Tweedie (1993)). Gain randomness through the jump or refreshment times.

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In soft/hard-sphere systems

- Dealing with diverging $\lambda \rightarrow$ control of a minimal distance
- Dealing with hardcore conditions $\rightarrow$ density condition ($\sim$ can pack $3N$ spheres of radius d_{pair}) (Metropolis algorithm, Diaconis, Lebeau, Michel (2011): linear)
- Dealing with periodicity and $e = +u_x, +u_y$

In soft/hard-sphere systems

- Dealing with diverging $\lambda \to$ control of a minimal distance > 0
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Strategy $x_0 \to x_f$

- Start in the case of well-separated spheres ($\min_{i \neq j}(d(x_{0,i}, x_{0,j}), d(x_{0,i}, x_{f,j}), d(x_{f,i}, x_{f,j})) > 2d_{\text{pair}}$) ($d$=periodic distance).
  Show the possibility to define a valid path only along $+u_x$ and $+u_y$ from any path along $\pm u_x, u_y$ which directly connects x_0 and x_f.

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  Careful with periodicity, no linear condition but use of hexagonal packing to exploit the existence of one separation of $4d_{\text{pair}}/\sqrt{3}$.

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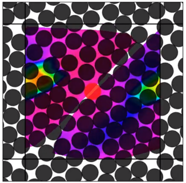
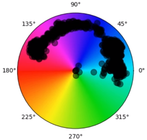
Can ease the dependence on x_0 (only travel times) for soft spheres.

Monemvassitis et al (2023)

Outline

Upgrading the deterministic flow





General flow: differential drift ϕ, $\phi_{t+s} = \phi_t \circ \phi_s$

$$\frac{\mathrm{d}(x_t, v_t)}{\mathrm{d}t} = \phi(x_t, v_t)$$

$$\int \mathcal{A}f(x,v)\mathrm{d}\pi(x)\mathrm{d}\mu(v) \to \int \mathrm{d}\pi(x)\mathrm{d}\mu(v) f(x,v)\nabla\cdot\phi(x,v) + \text{transport} + \text{events}$$

Vanetti et al (2017)

Rotational flow, ϕ_R: α- rotation of i-th sphere around a point at $x_i - l(\cos(\psi), \sin(\psi))$

$(x, v) = (x, \alpha, l, \psi)$ and $\phi(x, v) = (l(-\sin\psi, \cos\psi)), 0, 0, \alpha) \to \nabla \cdot \phi_R(x, v) = 0$

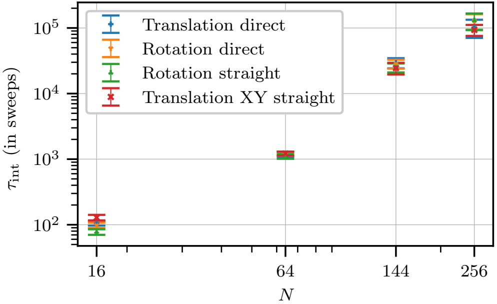
Hybrid flow: alternate between ϕ_R and ϕ_T depending on ω

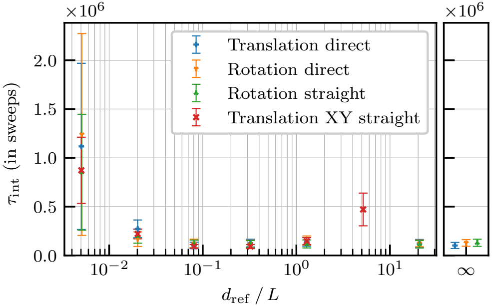
$(x, v) = (x, \omega, (e, i), \alpha, l, \psi)$ and

$\phi_H(x, v) = \omega(e, 0, 0, 0, 0) + (1 - \omega)(l(-\sin\psi, \cos\psi)), 0, 0, 0, \alpha) \to \nabla \cdot \phi_H(x, v) = 0$

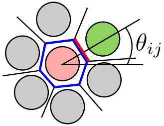
Guyon et al (2023)

Applications to hard disks - at hexatic density





Observable: ϕ_6, $N = 256$



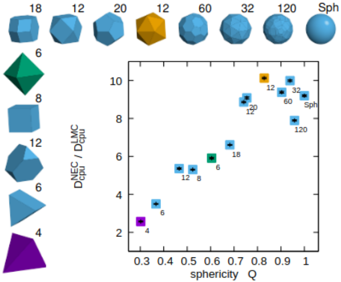
Guyon et al (2023)

Outline

Non-reversible sampling of anisotropic particles

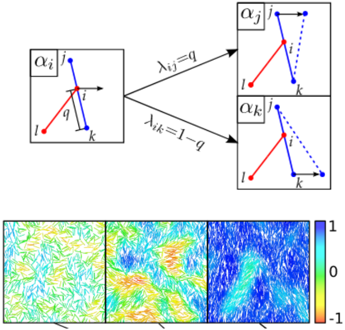
Without rotational flow

Hybrid Metropolis/ECMC



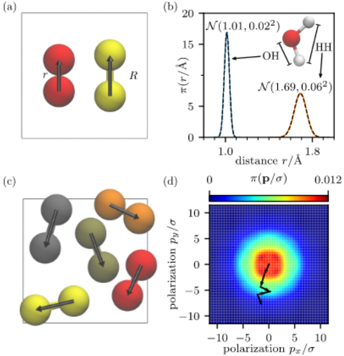
Klement et al (2021)

Elastic length



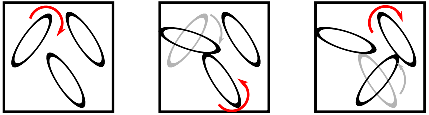
Harland et al (2017)

Tethered interaction

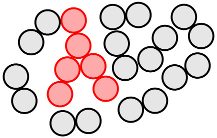


Höllmer et al (2021)

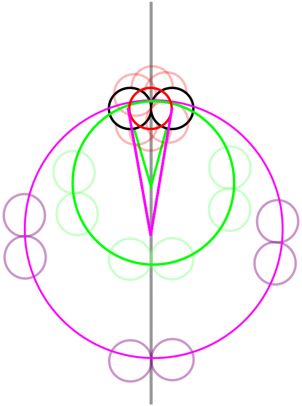
Rotations are necessary to thermalize dimers



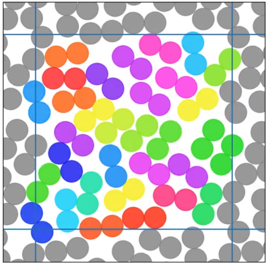
Self-Rotations cannot be naively propagated as translations, as breaking of symmetry:
$|\mathrm{d}_{R(i)} E_{ij}| \neq |\mathrm{d}_{R(j)} E_{ij}|$ in general



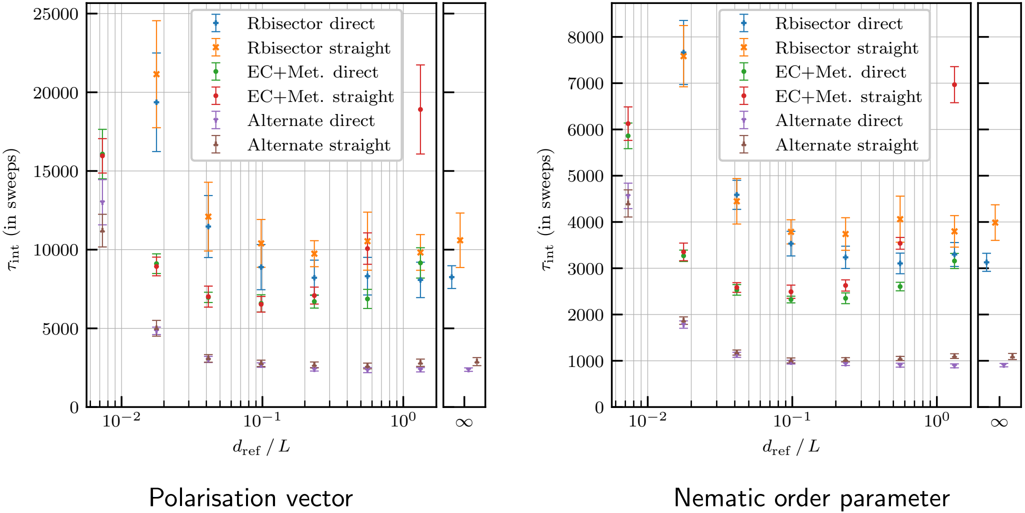
Bisector rotation



No backtracking!

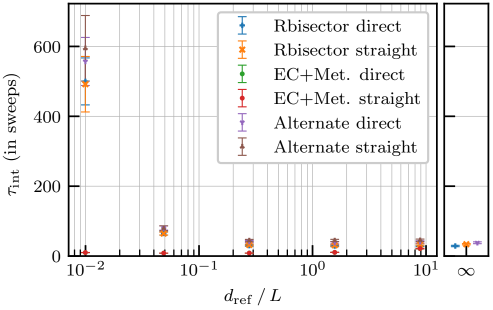


Numerical comparaison - (density $\rho = 0.7$, $N = 32$)

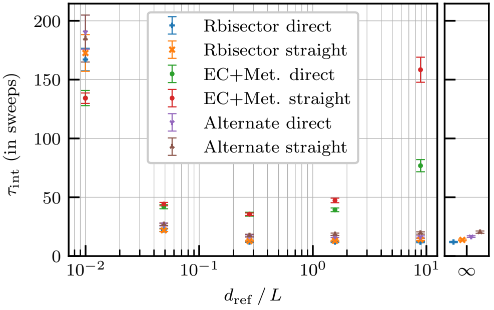


Guyon et al (2023)

Numerical comparaison - (density $\rho = 0.5$, $N = 32$)



Polarisation vector



Nematic vector order parameter

Guyon et al (2023)

Conclusion

Finding the entropic opening by building persistency into moves along PDMP

- Non-reversibility obtained by exploiting global symmetries
  - Flexible schemes based on the exploitation and (stochastic) control of a ballistic exploration of the state space.
  - The PDMP framework allows for a clear and direct formalism.
  - Generalisation to other flows than the translations, generalisation to the non-reversible sampling of anisotropic particle systems.

Some questions

- Ergodicity proof at relevant densities, with/without refreshment
- Trade off between generating persistent transport while avoiding building too strong correlations
- Still missing something in hard disks

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Finding the entropic opening by building persistency into moves along PDMP

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Thank you for your attention!

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ANR
SuSa

Joint work with Arnaud Guillin, Tristan Guyon, Athina Monemvassitis (UCA)

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