Speeding-up sampling with nonreciprocal interaction

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Roadmap

1. Why bother?
2. Irreversible samplers
3. One particle in a potential
4. Structural glasses: an introduction
5. Numerical exploration
6. Fluid in infinite dimensions
7. Mode coupling theory
8. Outlook

Setting up the stage

Consider a system with many degrees of freedom and energy V

Goal: sample Boltzmann, $e^{-\frac{V}{T}}$

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Hard in some interesting fields

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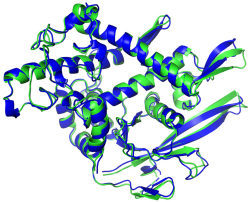

Protein folding
DeepMind

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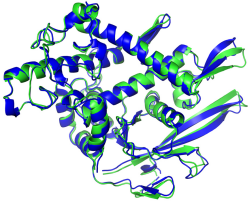

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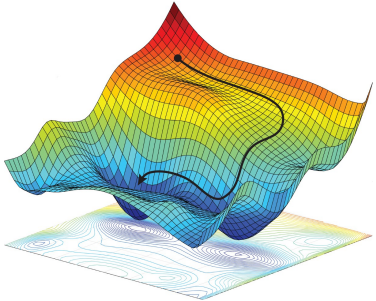

Machine Learning & Optimization
Amini *et al.*, NIPS (2017)

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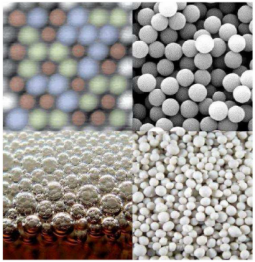

Disordered materials
Berthier & Biroli, RMP (2011)

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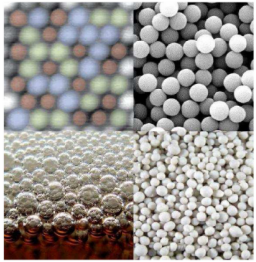

Disordered materials
Berthier & Biroli, RMP (2011)

PHYSICAL REVIEW X **12,** 041028 (2022)

Thirty Milliseconds in the Life of a Supercooled Liquid

Camille Scalliet,[1] Benjamin Guiselin,[2] and Ludovic Berthier[3,4,*]

Basic ingredients

Overdamped Brownian Dynamics

$$\dot{\mathbf{x}} = -\boldsymbol{\nabla} V(\mathbf{x}) + \sqrt{2T}\boldsymbol{\xi}$$

$$\left\langle \xi_i(t)\xi_j(t') \right\rangle = \delta_{ij}\delta(t-t')$$

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$$\begin{aligned} \partial_t \rho(\mathbf{x}, t) &= \boldsymbol{\nabla} \cdot [(\boldsymbol{\nabla} V)\rho + T\boldsymbol{\nabla}\rho] \\ &= -H_{\mathrm{FP}}\rho \end{aligned}$$

Basic ingredients

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$$\rho(\mathbf{x}, t) = \rho_\lambda(\mathbf{x})e^{-\lambda t} \quad H_{\mathrm{FP}}\rho_\lambda = \lambda\rho_\lambda$$

Basic ingredients

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Steady state equilibrium solution: $\rho_0 \propto \mathrm{e}^{-\frac{V}{T}} = \rho_{\mathrm{B}}$

Basic ingredients

$$\rho(\mathbf{x}, t) = \rho_\lambda(\mathbf{x})\mathrm{e}^{-\lambda t} \quad H_{\mathrm{FP}}\rho_\lambda = \lambda\rho_\lambda$$

V confining enough: λ_1 smallest, positive eigenvalue

$$\rho(\mathbf{x}, t) \approx \rho_{\mathrm{B}}(\mathbf{x}) + \phi_{\lambda_1}(\mathbf{x})e^{-\lambda_1 t}$$

Relaxation time

$$\tau_{\mathrm{R}} = \frac{1}{\lambda_1}$$

Basic ingredients

$$\mathscr{P}[\mathbf{x} \to \mathbf{x} + \mathrm{d}\mathbf{x} = \mathbf{x} + \dot{\mathbf{x}}\mathrm{d}t] \propto \rho_{\mathrm{B}}(\mathbf{x})\mathrm{e}^{-\frac{\mathrm{d}t}{4T}(\dot{\mathbf{x}}+\nabla V)^2}$$

Entropy production rate

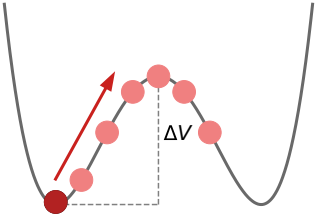
$$\dot{\Sigma} \equiv \int \mathrm{d}^d x \rho_{\mathrm{B}} \frac{1}{dt} \log \frac{\mathscr{P}[\mathbf{x} \to \mathbf{x} + \dot{\mathbf{x}}\mathrm{d}t]}{\mathscr{P}[\mathbf{x} + \dot{\mathbf{x}}\mathrm{d}t \to \mathbf{x}]}$$

Equiblibrium Brownian Dynamics: $\dot{\Sigma} = 0$

Basic ingredients

τ_R can become very large

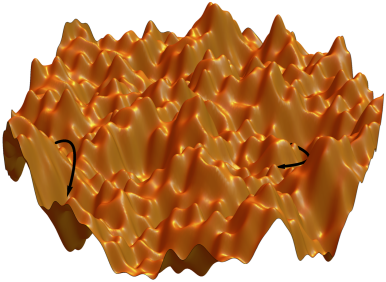
$$\dot{x} = -V'(x) + \sqrt{2T}\xi$$



$$\tau_R \propto e^{\frac{\Delta V}{T}}$$

Basic ingredients

τ_R can become very large



Can we reduce τ_R?

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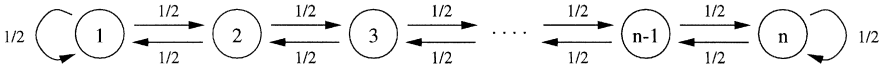
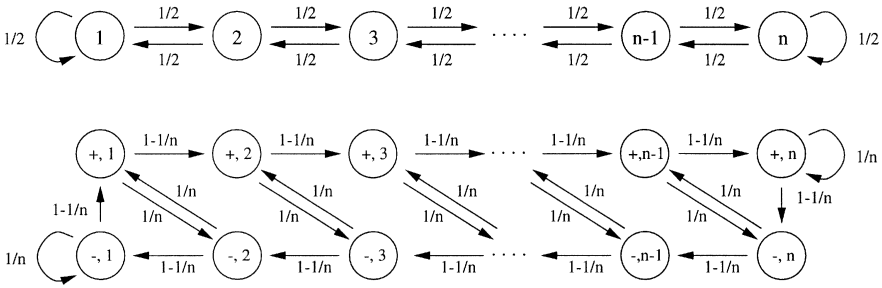
An insight from applied math



An insight from applied math



Diaconis *et al.*, Ann. App. Prob. 2000

Lifting: extra degrees of freedom + irreversible dynamics

An insight from computer science

Quantum Speed-up of Markov Chain Based Algorithms

Mario Szegedy*

An insight from computer science

Quantum Speed-up of Markov Chain Based Algorithms

Mario Szegedy*

Szegedy, 45th Annual IEEE symposium on Foundations of Computer Science (2004)

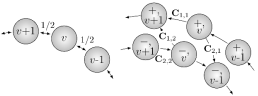


Figure 1: (left) random walk $\mathbf{P}_G$ on the N-cycle; (right) quantum walk unitary with coin toss $\mathbf{C}$, lifted Markov chain with a stochastic coin toss $\overline{\mathbf{C}}$, suggesting their comparison.

Apers *et al.*, Phys. Rev. A (2018)

Lifting or Coin toss: basically the same idea

From applied math to active particles

Lifting: extra degree of freedom + irreversible dynamics

$$\dot{\mathbf{x}} = -\mu \boldsymbol{\nabla} V(\mathbf{x}) + \sqrt{2T\mu}\boldsymbol{\xi} + \mathbf{v}$$

$$\rho_{ss}(\mathbf{x}, \mathbf{v}) \propto f(\mathbf{v}) e^{-\frac{V(\mathbf{x})}{T}}$$

Dynamics of $\mathbf{v} \rightarrow$ active samplers of Boltzmann: RTPs, AOUPs, ABPs...

From applied math to active particles

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Dynamics of $\mathbf{v} \rightarrow$ active samplers of Boltzmann: RTPs, AOUPs, ABPs...

From applied math to active particles

Intuition – Run and Tumble Particle
Uniform distribution over $[0, L]$

$$\dot{x} = v$$

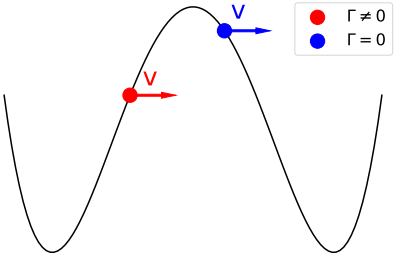
$$v = v_0 \times (\pm 1) \text{ at rate } \frac{1}{\tau}$$

$$\tau_{\text{first}}(L) = \frac{L}{v_0} + \frac{L^2}{v_0^2 \tau}$$

From applied math to active particles

Example 1 - Run and Tumble Particle

$$\dot{\mathbf{x}} = -\mu \boldsymbol{\nabla} V(\mathbf{x}) + \sqrt{2T\mu}\boldsymbol{\xi} + \mathbf{v}$$
$$\mathbf{v} = v_0 \mathbf{u}$$
$$\Gamma(\mathbf{u} \to \mathbf{u}') = v_0 \beta (\mathbf{u} - \mathbf{u}') \cdot \boldsymbol{\nabla} V \theta \left((\mathbf{u} - \mathbf{u}') \cdot \boldsymbol{\nabla} V \right)$$



From applied math to active particles

Example 2 - Lifted active Ornstein-Uhlenbeck

$$\dot{\mathbf{x}} = -\mu \nabla V + \mathbf{v} + \sqrt{2\mu T}\boldsymbol{\xi}$$

$$\dot{\mathbf{v}} = -\frac{1}{\tau}\mathbf{v} - \beta v_0^2 \nabla V + \sqrt{\frac{2v_0^2}{\tau}}\boldsymbol{\chi}$$

From active particles to non reciprocal interactions

Lifted AOUPs

$$\dot{\mathbf{x}} = -\mu \boldsymbol{\nabla} V + \mathbf{v} + \sqrt{2\mu T}\boldsymbol{\xi}$$

$$\dot{\mathbf{v}} = -\frac{1}{\tau}\mathbf{v} - \beta v_0^2 \boldsymbol{\nabla} V + \sqrt{\frac{2v_0^2}{\tau}}\boldsymbol{\chi}$$

Effective potential $U(\mathbf{x}, \mathbf{v}) \equiv \frac{\mathbf{v}^2}{2\beta v_0^2} + V(\mathbf{x})$

$$\begin{bmatrix} \dot{\mathbf{x}} \\ \dot{\mathbf{v}} \end{bmatrix} = - \begin{bmatrix} \mu & -\gamma \\ \gamma & v_0^2/\tau \end{bmatrix} \begin{bmatrix} \partial_{\mathbf{x}} U \\ \partial_{\mathbf{v}} U \end{bmatrix} + \text{noise}$$

with $\gamma = \beta v_0^2$

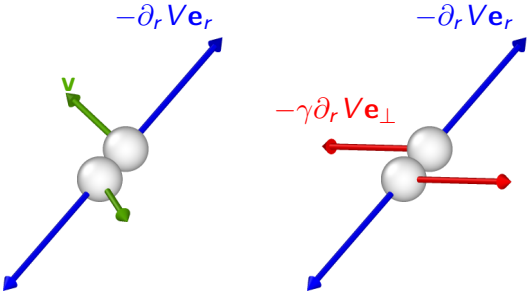
From active particles to non reciprocal interactions

$$\dot{\mathbf{r}} = -(\mathbb{1} + \gamma \mathbf{A})\boldsymbol{\nabla} V + \sqrt{2T}\boldsymbol{\xi} \quad \mathbf{A}^T = -\mathbf{A}$$

- $\rho_{ss} \propto e^{-\beta V}$
- Irreversible dynamics, $\dot{\Sigma} = \frac{\gamma^2}{2T} ||\mathbf{A}||_{\mathrm{F}}^2 \left\langle (\boldsymbol{\nabla} V)^2 \right\rangle$
- Nonreciprocal interaction among different degrees of freedom
- $\mathbf{A} \sim O(\mathbb{1}) \to \gamma$: strength of nonequilibrium drive

From active particles to non reciprocal interactions

Active particles, chirality and nonreciprocal interactions



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Non-Hermitian speed-up

$$H = H_0 + \gamma H_{\mathbf{A}}$$

$$H_0^\dagger = H_0 \qquad\qquad H_{\mathbf{A}}^\dagger = -H_{\mathbf{A}}$$

$$|\gamma| \ll 1$$

γ **real**

$$\delta\lambda_1 \approx \underbrace{i\gamma a_1}_{\text{imaginary}} + \underbrace{\gamma^2 a_2}_{\geq 0}$$

$$\tau_{\mathrm{R}}(\gamma) \leq \tau_{\mathrm{R}}(0)$$

Nonequilibrium speed-up

Entropy production rate $\dot{\Sigma} = \gamma^2 \langle (\boldsymbol{\nabla} V)^2 \rangle = \tau_{\Sigma}^{-1}$

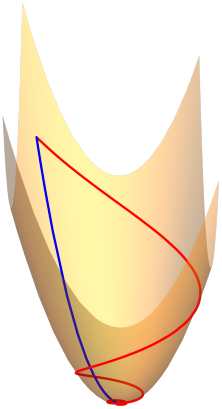
Dissipation proportional to activity, matters after a time τ_{Σ}

Harmonic well

$$V(\mathbf{r}) = \tfrac{1}{2}\mathbf{r}^2,\ \mathbf{A} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

$$\dot{\mathbf{r}} = -(\mathbb{1} + \gamma\mathbf{A})\mathbf{r} + \sqrt{2T}\boldsymbol{\xi}$$

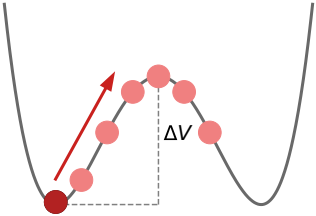
$$\boxed{\tau_{\mathrm{R}}(\gamma) = \tau_{\mathrm{R}}(0)}$$



Barrier crossing

$$\dot{x} = -V'_{\mathrm{dw}}(x) + \sqrt{2T}\xi$$

$$V_{\mathrm{dw}}(x) = \frac{1}{4}x^4 - \frac{1}{2}x^2$$



τ time needed to cross the barrier

At low T, $\tau = \frac{2\pi}{\sqrt{k_m K_M}} e^{\frac{\Delta V}{T}}$

Barrier crossing

We consider two copies of the same system with antisymmetric coupling[1]

$$\begin{bmatrix} \dot{x} \\ \dot{y} \end{bmatrix} = -(\mathbb{1} + \gamma \mathbf{A}) \begin{bmatrix} \partial_x U \\ \partial_y U \end{bmatrix} + \sqrt{2T}\boldsymbol{\xi}$$

$$\text{with } \mathbf{A} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \; U(x, y) = V_{\mathrm{dw}}(x) + V_{\mathrm{dw}}(y)$$

What is τ?

Path during barrier crossing ?

Difficulties: not a 1d problem + nonequilibrium drift

[1] Ichiki & Ohzeki, PRE 2015

Barrier crossing

$$\tau = \frac{2\pi}{|\lambda_+|}\sqrt{\frac{k_M}{k_m}}e^{\frac{\Delta V}{T}}$$

λ_+: positive eigenvalue of dynamics at the saddle point[2]
Our case[3]

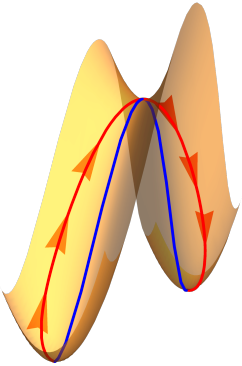
$$\lambda_+ = \frac{1}{2}\left[k_M - k_m + \sqrt{(k_M + k_m)^2 + 4\gamma^2 k_m k_M}\right] > k_M$$

$$\tau(\gamma) < \tau(0)$$

[2] Reygner & Bouchet, Ann. H. Poincaré 2016
[3] Ghimenti, Van Wijland PRE 2022

Barrier crossing

$$\dot{\mathbf{x}}_{\text{path}} = (\mathbb{1} - \gamma \mathbf{A})\, \nabla U(\mathbf{x}_{\text{path}})$$



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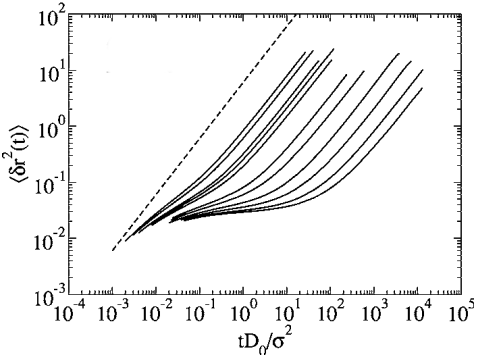
Dense fluids with nonreciprocal interactions

$$
\begin{aligned}
\dot{\mathbf{r}}_i &= (\mathbb{1} + \gamma \mathbf{A})\mathbf{F}_i + \sqrt{2T}\boldsymbol{\xi}_i \\
\mathbf{A}^T &= -\mathbf{A} \\
\mathbf{F}_i &\equiv -\sum_{j \neq i} \boldsymbol{\nabla} V(|\mathbf{r}_i - \mathbf{r}_j|)
\end{aligned}
$$

Motion in real space

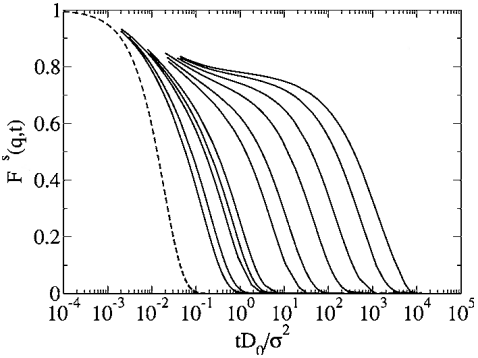
$$\left\langle \delta r^2(t) \right\rangle \equiv \frac{1}{N} \sum_i \left\langle [\mathbf{r}_i(t) - \mathbf{r}_i(0)]^2 \right\rangle \xrightarrow{t \to \infty} 2dDt$$



Flenner & Szamel, PRE 2005

Motion in reciprocal space

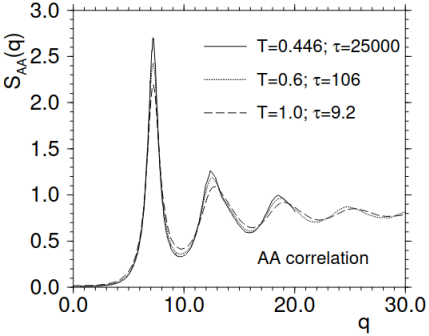
$$F^S(\mathbf{q}, t) \equiv \left\langle \frac{1}{N} \sum_j e^{-i\mathbf{q}\cdot[\mathbf{r}_i(t)-\mathbf{r}_i(0)]} \right\rangle$$



Flenner & Szamel, PRE 2005

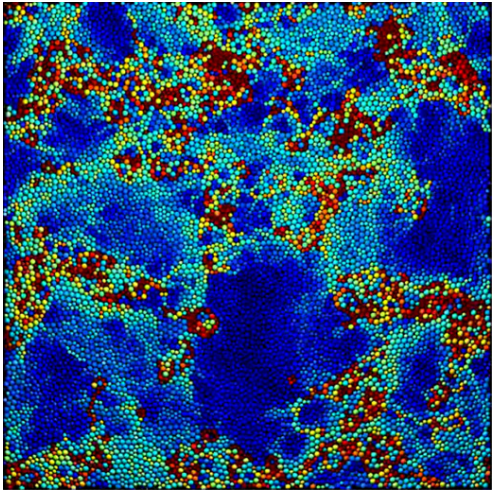
Structural properties

$$S(\mathbf{q}) = \frac{1}{N} \left\langle \sum_{i,j} e^{-i\mathbf{q}\cdot[\mathbf{r}_i - \mathbf{r}_j]} \right\rangle$$

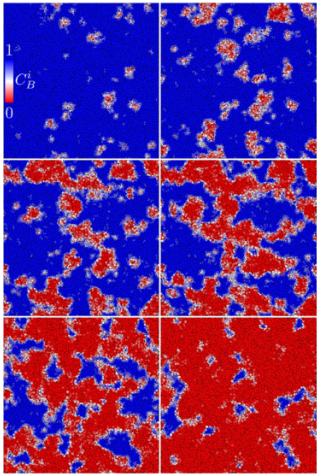


Kob, Les Houches 2002

Dynamical hetereogenities and simulations



Keys *et al.* PRX 2011



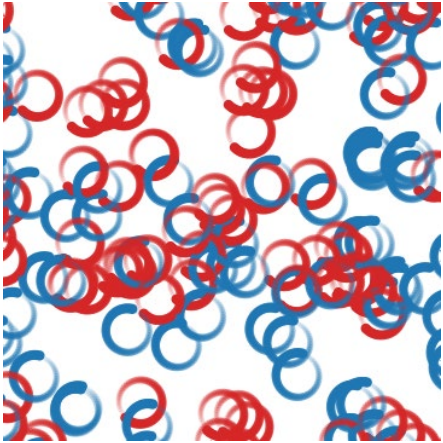
Scalliet *et al.* PRX 2022

The many temperatures of the glass transition

- $\mathbf{T_o}$: $\tau_\alpha \neq \exp \frac{C}{T}$
- $\mathbf{T_g}$: Plateau of F^s goes beyond experimental timescale
- $\mathbf{T_d}$: $\lim_{t\to\infty} F^s(q,t) = f_0 \neq 0$. Avoided in finite dimension
- $\mathbf{T_c}$: Thermodynamic transition, a stable glass (paradigm: mean field)

Our focus: Systems displaying $\mathbf{T_d}$

Odd transport



Hanai *et al.*, Nature 2021

Odd transport

Odd diffusivity[4]

$$D_\perp = \frac{1}{N}\sum_{i=1}^{N}\int_0^{+\infty} dt\, \langle \dot{\mathbf{r}}_i(t)\cdot \boldsymbol{A}\dot{\mathbf{r}}_i(0)\rangle$$

[4] Hargus *et al.*, PRL 2021

Odd transport

$$\eta_{abcd} = \frac{\beta}{V}\int_0^{+\infty} dt \left\langle \sigma^{\mathrm{IK}}_{cd}(t)(\mathbb{1} + \gamma \mathbf{A})_{be}\sigma^{\mathrm{IK}}_{ae} \right\rangle \quad \sigma^{\mathrm{IK}}_{ab} = \frac{1}{2}\sum_{i\neq j} r_{ij,a}F_{ij,b}$$

Odd viscosity[5]

$$\eta_{\perp} \equiv \eta_{xxxy} - \eta_{xyxx}$$

[5] Banerjee *et al.*, Nature 2017

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Numerical exploration

Binary Kob-Andersen mixture [6]

$$\dot{\mathbf{r}}_i = -\beta D_0 \sum_{j \neq i} (\mathbb{1} + \gamma \mathbf{A}) \boldsymbol{\nabla} V_{\alpha_i,\alpha_j}(|\mathbf{r}_i - \mathbf{r}_j|) + \sqrt{2D_0}\boldsymbol{\xi}_i$$

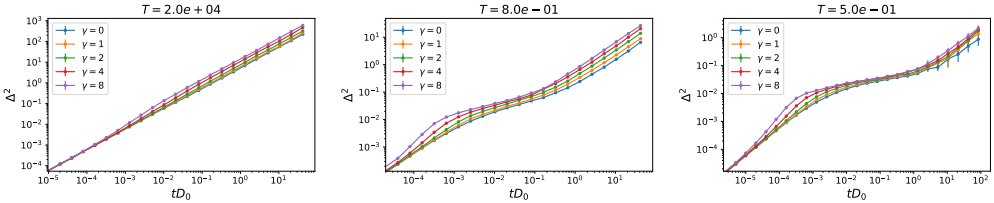
$$V_{\alpha\beta}(r) = 4\epsilon_{\alpha\beta}\left[\left(\frac{\sigma_{\alpha\beta}}{r}\right)^{12} - \left(\frac{\sigma_{\alpha\beta}}{r}\right)^{6}\right], \mathbf{A} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

[6] Kob & Andersen, PRE 1995

Numerical exploration

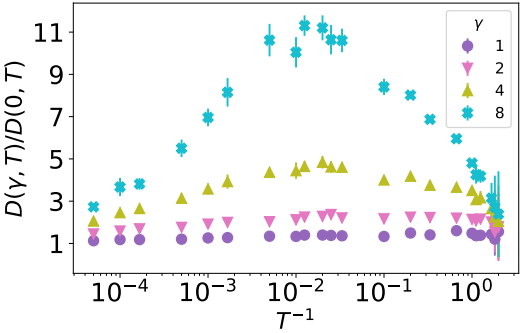
$$\Delta^2(t) \equiv \frac{1}{N}\sum_{i=1}^{N_A}\left\langle [\mathbf{r}_i(t) - \mathbf{r}_i(0)]^2 \right\rangle$$

$$\gamma = \mathbf{0} : \rho = 1.2,\ T_d = 0.435$$



Numerical exploration

$$D \equiv \lim_{t\to\infty} \frac{\Delta(t)}{2dt}$$

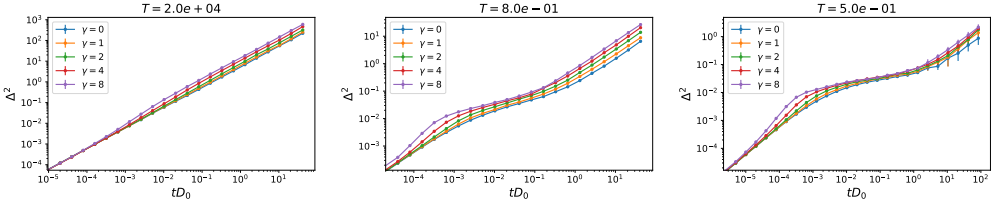


Can we rationalize this result?

Numerical exploration

$$\Delta^2(t) \equiv \frac{1}{N}\sum_{i=1}^{N_A}\left\langle [\mathbf{r}_i(t) - \mathbf{r}_i(0)]^2 \right\rangle$$

$$\gamma = \mathbf{0} : \rho = 1.2,\ T_d = 0.435$$



Numerical exploration

$$D_\perp = \int_0^{+\infty} \langle \dot{x}_i(t) y_i(0) - \dot{y}_i(t) x_i(0) \rangle \mathrm{d}t$$

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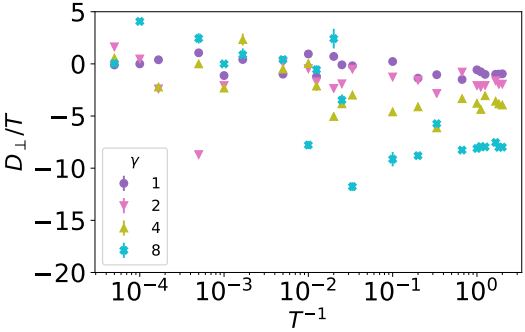

Can we rationalize this result too?

Roadmap

1. Why bother?
2. Irreversible samplers
3. One particle in a potential
4. Structural glasses: an introduction
5. Numerical exploration
6. **Fluid in infinite dimensions**
7. Mode coupling theory
8. Outlook

Infinite dimensional fluid

A system of interacting particle in $d \to \infty$ dimension

$$\zeta \dot{\mathbf{r}}_i = (\mathbb{1} + \gamma \mathbf{A})\mathbf{F}_i + \sqrt{2T\zeta}\boldsymbol{\xi}_i$$
$$\mathbf{F}_i = -\sum_i \boldsymbol{\nabla} V(|\mathbf{r}_i(t) - \mathbf{r}_j(t)|)$$

No time to address during the live presentation!

Oral summary: Results consistent with the simulations.

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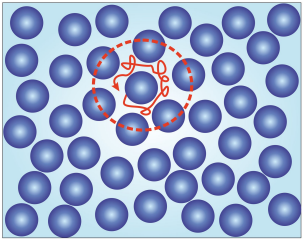
Mode coupling theory

$$\dot{\mathbf{r}}_i = D_0\beta(\mathbb{1} + \gamma\mathbf{A})\mathbf{F}_i + \sqrt{2D_0}\boldsymbol{\xi}_i$$

$$\mathbf{F}_i = -\sum_{j\neq i} \boldsymbol{\nabla} V(|\mathbf{r}_i - \mathbf{r}_j)$$

$$\mathbf{A} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

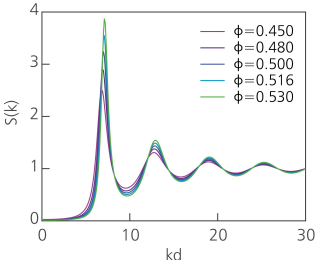


Mode coupling theory

Input

Static structure factor

$$S(\mathbf{k}) \equiv \frac{1}{N} \left\langle \sum_{i,j} e^{-i\mathbf{k}\cdot[\mathbf{r}_i - \mathbf{r}_j]} \right\rangle$$



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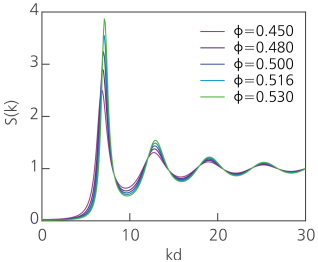
Mode coupling theory

Input

Static structure factor

$$S(\mathbf{k}) \equiv \frac{1}{N} \left\langle \sum_{i,j} e^{-i\mathbf{k}\cdot[\mathbf{r}_i - \mathbf{r}_j]} \right\rangle$$



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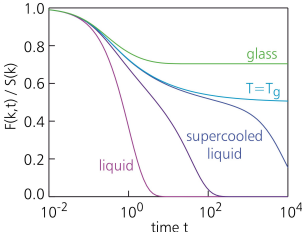
Output

Dynamical structure factor

$$F(\mathbf{k}, t) \equiv \frac{1}{N} \left\langle \sum_{i,j} e^{-i\mathbf{k}\cdot[\mathbf{r}_i(t) - \mathbf{r}_j(0)]} \right\rangle$$



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Oral summary: Consistent with simulations.

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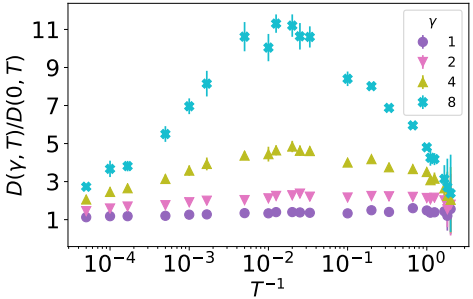
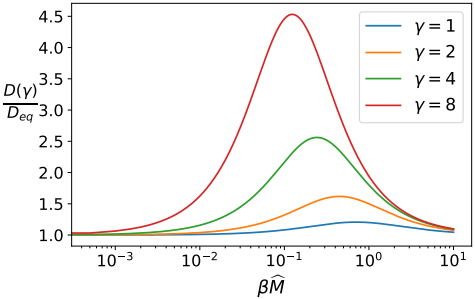
Outlook





- Generalised Mode Coupling theory?
- Acceleration below the MCT crossover?
- Numerical feasibility: Monte Carlo implementations?
- Sorting out ingredients (rescaling, memory, irreversibility)