Efficiency of transverse forces in dense systems

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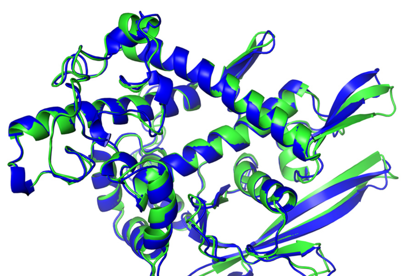
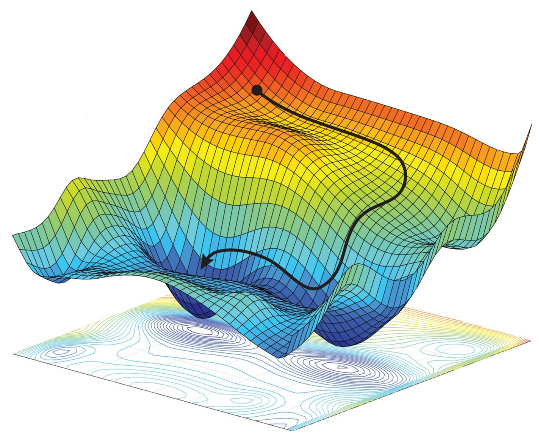
1. Sampling Boltzmann

The goal: $\rho_B \propto e^{-\beta V}$

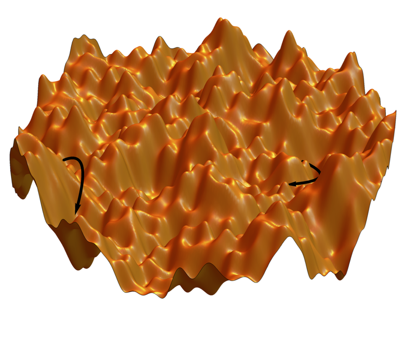
Hard in some relevant cases



DeepMind



Amini, NIPS 2017



C. Cammarota

Equilibrium sampling

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

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

$$\partial_t \rho(\mathbf{r},t) = -\nabla\cdot\mathbf{j}(\mathbf{r},t)$$

$$\rho(\mathbf{r},t) \approx \rho_{\mathrm{B}}(\mathbf{r}) + e^{-\frac{t}{\tau_{\mathrm{R}}}}\phi_1(\mathbf{r})$$

τ_{R} can become very large ... new dynamical rules?

2. Transverse Forces

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

$$\mathbf{A}^T = -\mathbf{A},\ \mathbf{A} \sim O(\mathbb{1})$$

Extra current $\partial_t\rho(\mathbf{r},t) = -\nabla\cdot\left(\mathbf{j}(\mathbf{r},t) + \mathbf{j}_\gamma(\mathbf{r},t)\right)$.

Sampling Boltzmann: $\nabla\cdot\mathbf{j}_\gamma(\mathbf{r},t) = 0$ when $\rho(\mathbf{r},t) = \rho_{ss}(\mathbf{r}) = \rho_{\mathrm{B}}$

Out of equilibrium: Entropy production rate $\dot{\Sigma} = \frac{\gamma^2}{T}\langle(\nabla V)^2\rangle > 0$

A theorem on dynamics' acceleration [1]

$$\tau_{\mathrm{R,irr}} \le \tau_{\mathrm{R,rev}}$$

How big is the speedup in dense fluids?

3. Connection with other schemes

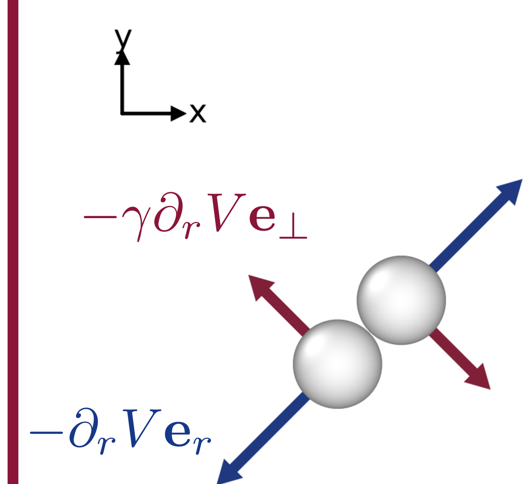
Ichiki-Ohzeki [2] Two copies of the same system

$$\mathbf{r} = (\mathbf{r}^{(1)}, \mathbf{r}^{(2)}),\ U(\mathbf{r}) = V(\mathbf{r}^{(1)}) + V(\mathbf{r}^{(2)})$$

$$\begin{bmatrix}\dot{\mathbf{r}}^{(1)}\\ \dot{\mathbf{r}}^{(2)}\end{bmatrix} = -\begin{bmatrix}\mathbb{1} & -\gamma\mathbb{1}\\ \gamma\mathbb{1} & \mathbb{1}\end{bmatrix}\cdot\begin{bmatrix}\nabla_{\mathbf{r}^{(1)}}U\\ \nabla_{\mathbf{r}^{(2)}}U\end{bmatrix} + \sqrt{2T}\begin{bmatrix}\boldsymbol{\xi}^{(1)}\\ \boldsymbol{\xi}^{(2)}\end{bmatrix}$$

- One can couple any two arbitrary systems
- An extended phase space with irreversible dynamics → **lifting** [3]

4. Transverse forces in dense liquids



$$\frac{\mathrm{d}\mathbf{r}_i}{\mathrm{d}t} = \mathbf{F}_i + \sqrt{2T}\boldsymbol{\xi}_i$$

$$\mathbf{F}_i = -(\mathbf{1} + \gamma\mathbf{A})\sum_{j\neq i}\nabla_{\mathbf{r}_i}V(|\mathbf{r}_i - \mathbf{r}_j|)$$

- Numerical simulations of structural glass-former
- Infinite dimensions
- Mode Coupling Theory

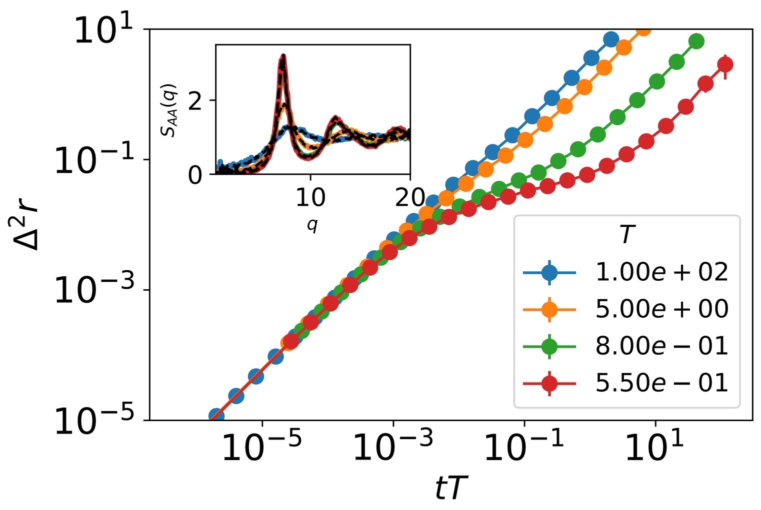
5. Numerics - Speedup

Brownian Dynamics simulations of a three dimensional 80:20 Kob-Andersen mixture [4, 5], $\mathbf{A} = \begin{bmatrix}0 & -1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 0\end{bmatrix}$

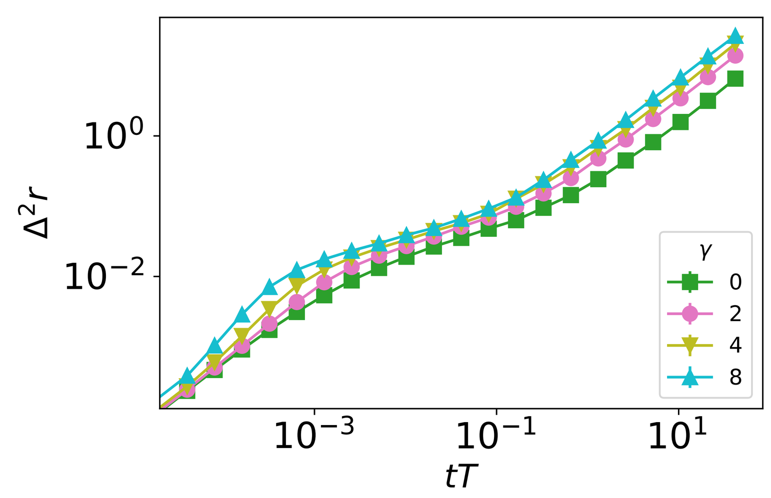
For $\gamma = 0$, $T \sim 1$ onset of slow dynamics

Structure: $S_{AA}(q) \equiv \frac{1}{N_A}\left\langle\sum_{i,j}^{N_A} e^{i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)}\right\rangle$

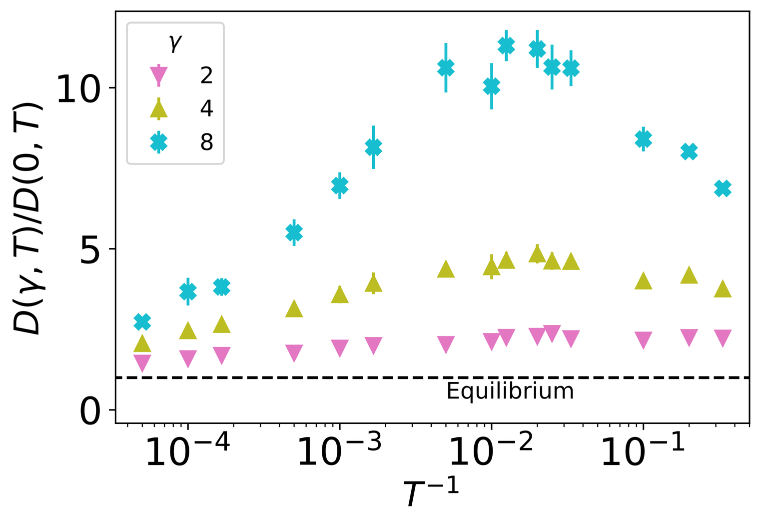
Dynamics: $\Delta^2 r(t) \equiv \frac{1}{N_A}\left\langle\sum_i^{N_A}[\mathbf{r}_i(t) - \mathbf{r}_i(0)]^2\right\rangle \overset{t\to\infty}{\approx} 6D(T,\gamma)t$



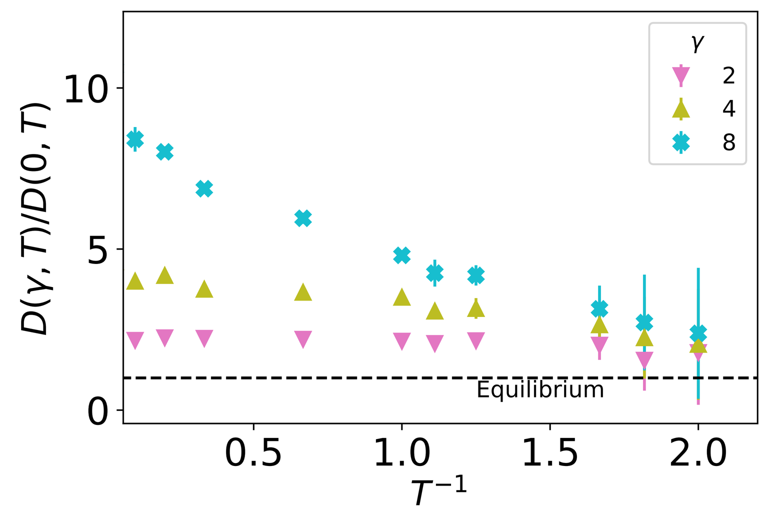
Calibration



A first glance at the speedup, T=0.8

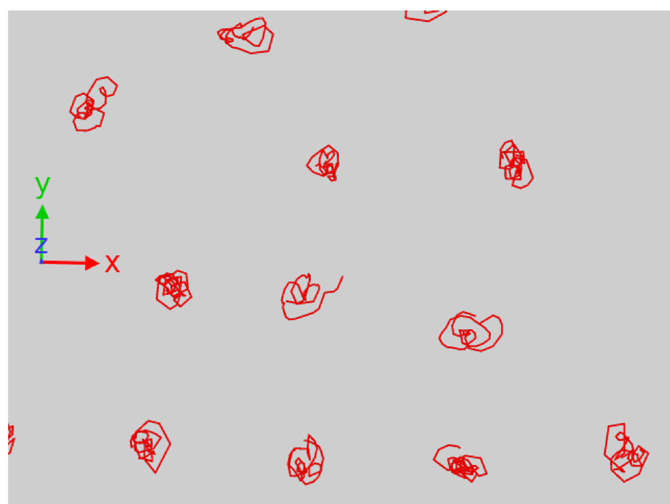


Maximal efficiency at **high T**



Efficiency **decreases** in the glass

6. Numerics - Odd transport



short time trajectories, $\gamma = 200$, $T = 0.8$

Motivation: odd diffusion helps relaxation [6]

$$D_\perp \equiv \frac{1}{2N_A}\sum_i^{N_A}\int_0^{+\infty} dt\,\langle\dot{\mathbf{r}}_i(t)\cdot\mathbf{A}\dot{\mathbf{r}}_i(0)\rangle$$

As T decreases, $D_\perp \to c(\gamma)$

Swirling without relaxing

7. Infinite dimensions

$$D(\gamma,T) = T\frac{1 + (1+\gamma^2)\beta\widehat{M}}{(1+\beta\widehat{M})^2 + (\gamma\beta\widehat{M})^2}$$

$$D_\perp(\gamma,T) = -\gamma T\frac{\beta\widehat{M} + (1+\gamma^2)(\beta\widehat{M})^2}{(1+\beta\widehat{M})^2 + (\gamma\beta\widehat{M})^2}$$

$\widehat{M} = \frac{1}{d}\int_0^{+\infty}\langle\nabla V(t)\cdot\nabla V(0)\rangle$, $\widehat{M}\to\infty$ for $T \to T_d(\gamma) = T_d(0)$

- $\mathbf{T} \to +\infty$: $D(\gamma,T)/D(0,T) = 1$, $D_\perp(\gamma,T) = 0$
- $\mathbf{T} \to \mathbf{T_d}$: $D(\gamma,T)/D(0,T) = a(\gamma)$, $D_\perp(\gamma,T) = -\gamma T$

Similar results for Mode Coupling Theory

8. Outlook

- Efficiency decreases when sampling gets harder
- Need for currents informed about the relevant degrees of freedom
- Monte Carlo schemes?

[1] C. Hwang, S. Hwang-Ma, and S. Sheu. *Ann. App. Prob.*, 1993.

[2] M. Ohzeki and A. Ichiki. *PRE*, 92(1):012105, 2015.

[3] M. Vucelja. *Am. J. Phys.*, 84(12), 2016.

[4] W. Kob and H. C Andersen. *PRE*, 51(5):4626, 1995.

[5] W. Kob and H. C Andersen. *PRE*, 52(4):4134, 1995.

[6] E. Kalz *et al.* *PRL*, 129(9):090601, 2022.