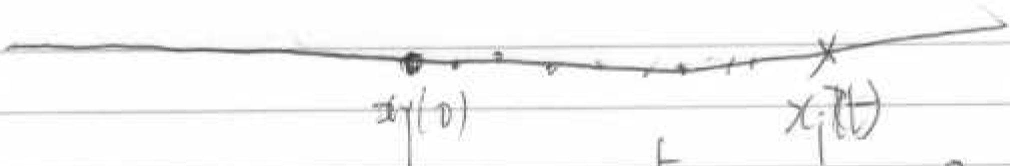
On the connection between single file dynamics and collective dynamics.

Single file dynamics: particles in a channel that cannot pass each other. Applications in biology and chemistry (flow through pores in a membrane, zeolites) traffic flows etc.

Tagged particle ~~transp~~ dynamics closely related to collective transport, as first noticed by Alexander and Pincus (PRB 18, 2011 (1978)))



$$\langle (x_j(t) - x_j(0))^2 \rangle \approx \frac{1}{n^2} \left\langle \left(\int_0^t d\tau \, j(0,\tau) \right)^2 \right\rangle$$

Warning: only correct in (average) rest frame of tagged particle. In moving frame $\langle \Delta^2(t) \rangle = v^2 t^2 + \langle \Delta_0^2(t) \rangle$ but fluctuations in $\int j\, dt$ increase.

To leading order:

$$\frac{\partial n(x,t)}{\partial t} = -\frac{\partial}{\partial x} j(x,t)$$

$$\frac{\partial \hat{n}(k,t)}{\partial t} = -ik\, \hat{j}(k,t)$$

$$\int_0^t d\tau\, \hat{j}(k,\tau) = -\frac{\left(\hat{n}(k,t) - \hat{n}(k,0)\right)}{ik} \quad (k \neq 0)$$

$$k=0: \int_0^t d\tau\, \hat{j}(0,\tau) = N\left(X(t) - X(0)\right)$$

$$\Rightarrow \left\langle \left(x_j(t) - x_j(0)\right)^2 \right\rangle = \frac{1}{n^2 L^2} \left\{ \sum_{k \neq 0} \frac{\left\langle \left(\hat{n}(k,t) - \hat{n}(k,0)\right)\left(\hat{n}(-k,t) - \hat{n}(-k,0)\right) \right\rangle}{k^2} \right.$$

$$+ \frac{N^2 \left\langle \left(X(t) - X(0)\right)^2 \right\rangle}{n^2 L^2}$$

$$= \sum_{k \neq 0} \frac{2S(k) - \left(S(k,t) + S(-k,t)\right)}{N n k^2} + \left\langle \left(X(t) - X(0)\right)^2 \right\rangle$$

with $S(k,t) \equiv \dfrac{\langle \hat{n}(k,t)\, \hat{n}(-k,0) \rangle}{L}$

In $\lim_{L \to \infty}$:

$$\langle (x_j(t) - x_j(0))^2 \rangle = \frac{1}{2\pi} \int dk \; \underbrace{\frac{2S(k) - (S(k,t) + S(-k,t))}{n^2 k^2}}_{\text{in "rest frame"}}$$

$+ \underbrace{V^2 t^2}$ (fluctuating part of $\langle (X(t) - X(0))^2 \rangle$ vanishes

to be added by hand if one wants expression in moving frame

Simplest category: dynamics of independent particles that exchange identity on crossing (equivalent: what is MSD of 137^{th} particle in the row?)

In that case: $S(k,t) = n\, S_{single}(k,t)$

suppose $S(k,t) = S(k)\, f(kt^{1/\alpha})$

$$\Rightarrow \langle (x_{free}(t) - x_{free}(0))^2 \rangle = -\left(\frac{\partial^2 S(k,t)}{\partial k^2}\right)_{k=0} \sim t^{2/\alpha}$$

but $\langle (x_j(t) - x_j(0))^2_{sf} \rangle \sim t^{1/\alpha}$ [provided $V=0$]

[Percus rule]

Examples:

1) Jepsen gas. Equal mass point particles, which exchange velocities on colliding

$$S(k,t) = \left\langle \frac{1}{L} \sum_{j\ell} e^{ik(x_j(0) - x_\ell(t))} \right\rangle$$

$$= \frac{N}{L} \left\langle \sum_j e^{-ikv_j t} \right\rangle = n \int dv\, \varphi(v)\, e^{-ikvt}$$

$$\Rightarrow \langle (x_j(t) - x_j(0))^2 \rangle = \frac{\langle |V| t \rangle}{n}$$

2) Non-crossing Brownian particles (T.E. Harris)

Now $S(k,t) = n e^{-Dk^2 t}$

$$\langle (x_j(t) - x_j(0))^2 \rangle = \frac{1}{\pi n} \int dk \, \frac{1 - e^{-Dk^2 t}}{k^2}$$

$$= \frac{2}{n} \sqrt{\frac{Dt}{\pi}}$$

For Brownian particles with drift: add $(Vt)^2$

3) Lévy flights: random flights with power law jump length distribution

$$S(k,t) = n e^{-\mathcal{D}|k|^\alpha t}$$

$$\langle (x_j(t) - x_j(0))^2 \rangle = \frac{1}{\pi n} \int dk \, \frac{1 - e^{-\mathcal{D}|k|^\alpha t}}{k^2}$$

requires $\alpha > 1$ for convergence

$$= \Gamma\left(\frac{\alpha - 1}{\alpha}\right) (\mathcal{D} t)^{1/\alpha}$$

$$\lim_{N\to\infty} \frac{N!}{n!\,(N-n)!}\left(\frac{\varepsilon}{N}\right)^n = \frac{\varepsilon^n}{n!}$$

$$p(m) = \sum_n \frac{\varepsilon^{2m+n}}{(m+n)!\; n!}$$

$$\simeq \sum \frac{\varepsilon^{2m+n}\, e^{m+2n}}{(m+n)^{m+n}\; n^n}$$

$$\log \frac{\varepsilon^n}{n!} = n \log\left(\frac{\varepsilon e}{n}\right)$$

$$\frac{\partial}{\partial n} = \log\left(\frac{\varepsilon e}{n}\right) - 1 \qquad = 0 \quad \text{for } n = \varepsilon$$

$$\frac{\partial^2}{\partial n^2} = -\frac{1}{n}$$

Gaussian distribution of displacement in AP approximation, for long times

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right of origin very large number of identically distributed particles, all having same probability $\sim t^{1/\alpha}$ of having crossed the origin.

Central limit theorem $\Rightarrow$ $n_{+-}(t)$ has Gaussian distribution with average $\sim t^{1/\alpha}$ and variance two

Same for $n_{-+}(t)$ $\Rightarrow$ $n_{+-} - n_{-+}$ also Gaussian, with average zero and variance $\sim t^{1/\alpha}$

Second category: interacting systems

AP approximation remains valid, but variety of possibilities becomes richer.

A few examples:

SEP Collective density satisfies diffusion equation $\Rightarrow$ same result for MSD as for independent BM

ASEP + other systems satisfying Fluct. Burgers eq.:

$$\frac{\partial n}{\partial t} = -\frac{\partial}{\partial x}\left(n\, u(n)\right) + D\frac{\partial^2 n}{\partial x^2} - \frac{\partial j_L}{\partial x}$$

Expand $u(n) = \bar{u} + (n-\bar{n})\overline{\frac{\partial u}{\partial n}} + \dots$

$$\Rightarrow \frac{\partial \delta n}{\partial t} = -\underbrace{\left(\bar{u} + \bar{n}\left(\frac{\partial \bar{u}}{\partial n}\right)\right)}_{\text{pattern velocity}}\frac{\partial \delta n}{\partial x} + \left\{\left(\frac{\partial u}{\partial n}\right) + \frac{\bar{n}}{2}\left(\frac{\partial^2 u}{\partial n^2}\right)\right\}\frac{\partial (\delta n)^2}{\partial x} + D\frac{\partial^2 n}{\partial x^2} - \frac{\partial j_L}{\partial x}$$

average drift velocity equals $\bar{u}$!

$$\Rightarrow \underset{\substack{\Downarrow \\ \text{in particle frame}}}{S(k,t)} = S(k,0)\, e^{-ik\bar{n}\left(\frac{\partial u}{\partial n}\right)t} \underset{\text{KPZ - scaling}}{f(k t^{2/3})}$$

For large t $\quad e^{-ik\ldots t}$ dominates

$$\Rightarrow \int dk \; \frac{2 - S(k,t) - S(-k,t)}{k^2} \sim t$$

(Notice: pattern velocity $\neq$ CM velocity)

Possible getting drift speed = pattern velocity?
Not with one species. But one may add
mutually non-passing second-class particles and
tune their jump rates. Should give MSD $\sim t^{2/3}$.

Hamiltonian dynamics

1d hamilt. systems with short-ranged interactions have

$$S(k,t) = \sum_{\sigma=\pm} S^{\sigma}(k,t) + S^{H}(k,t)$$

$$S^{\sigma}(k,t) = e^{-i\sigma c k t} f_{KPZ}(k t^{2/3})$$

$$S^{H}(k,t) = e^{-\alpha k^{5/3} t} \quad \text{[like Lévy flights]}$$

$\Rightarrow$ 3 contributions to MSD:

$$S^{\sigma} \Rightarrow ct$$

$$S^{H} \Rightarrow t^{3/5}$$

Finite size effects

① Hamilt. systems with fixed CM and PBC

1) Due to fixed CM the $k=0$ term in summation over k vanishes. So one misses $\langle V_{cm}^2 \rangle t^2$.

2) Plus, fixing CM constrains displacement of a single particle to $\frac{N-1}{N} L$ $\leftarrow$ (??)

$\Rightarrow$ MSD saturates for long times

Results Pooch

3) AP approximation ignores effects of systematic and stochastic deviations from fixed interparticle intervals.

Can be calculated for $t \to \infty$

$$\langle (x_j(t) - x_j(0))^2 \rangle = \langle (x_j(t) - \langle x_j \rangle - (x_j(0) - \langle x_j \rangle))^2 \rangle$$
$$= 2 \langle (x_j - \langle x_j \rangle)^2 \rangle$$

x_j from equidistant configuration with same CM position

Diffusive systems with PBC

For long times CM performs diffusive motion with $D_{CM} = \frac{D}{N}$

Tagged particle:

$$\langle (x_j(t) - x_j(0))^2 \rangle = \langle (x_j(t) - \langle x_j(t) \rangle - (x_j(0) - \langle x_j(0) \rangle))^2 \rangle$$

$$= \langle (X(t) - X(0))^2 \rangle + 2 \langle (x_j - \langle x_j \rangle)^2 \rangle$$

So for large t differs from Hamiltonian result by additional $\frac{2Dt}{N}$ only!

Attention for meeting on SFD in Erice from July 4-9, organized by Ophir Flomenbom, see

singlefiledynamicsconference.net

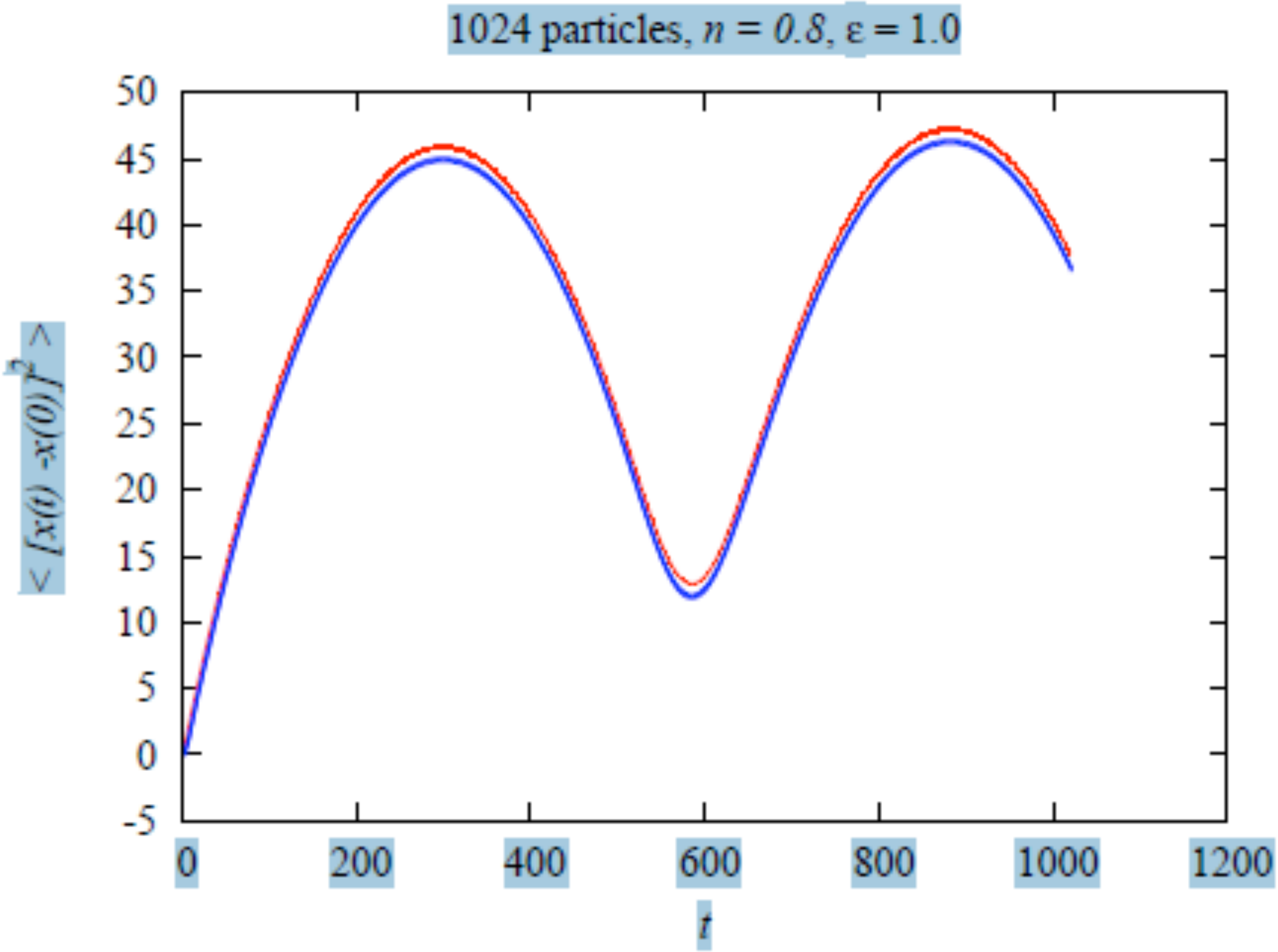

FIG. 2: Comparison of mean-squared deviation (MSD) (with error bars) for $N = 1024$.
Red: simulation value; blue: Alexander-Pincus approximation based on simulation values for S(k,t)

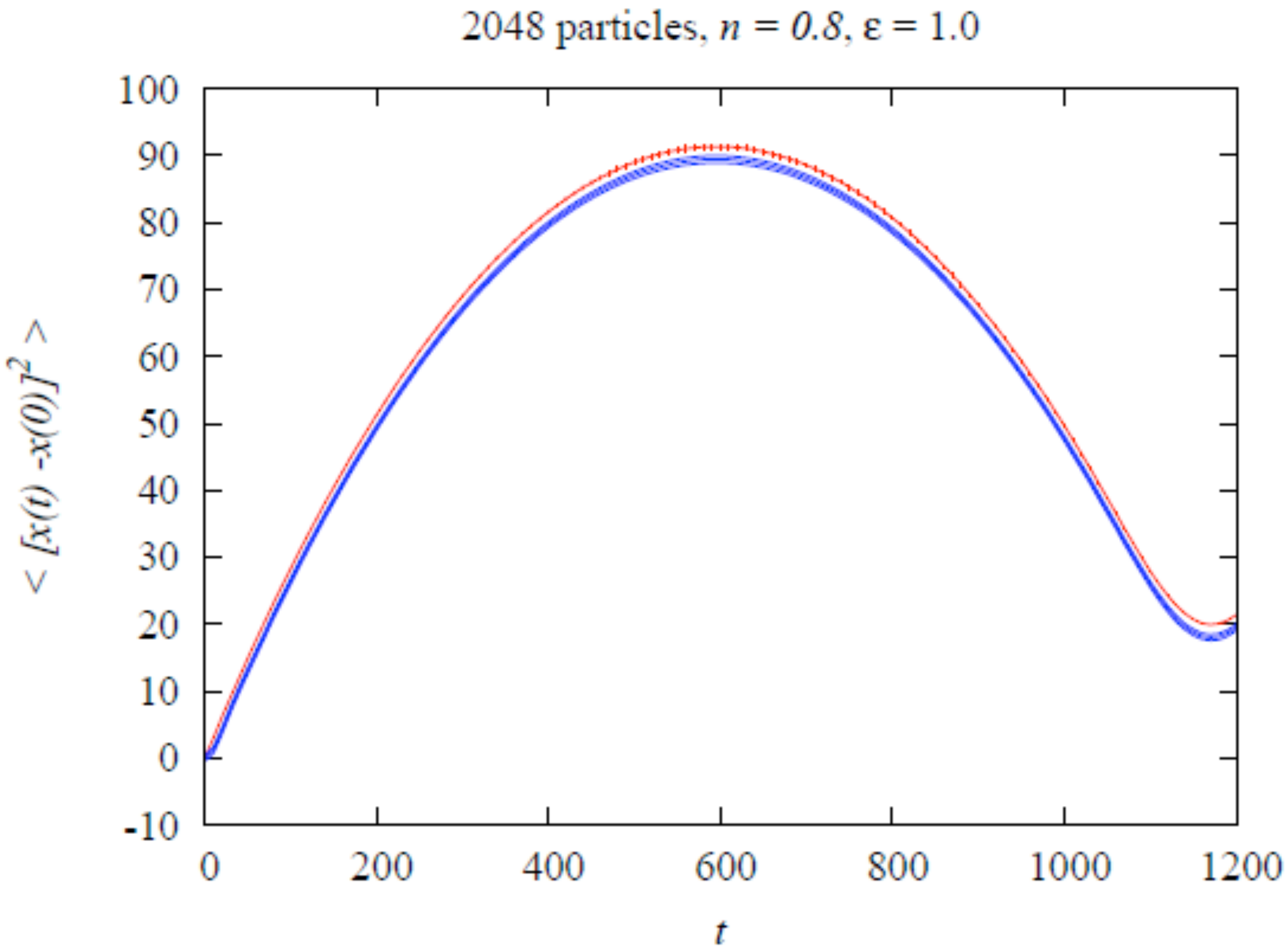

FIG. 3: Comparison of mean-squared deviation MSD (with error bars) for $N = 2048$.

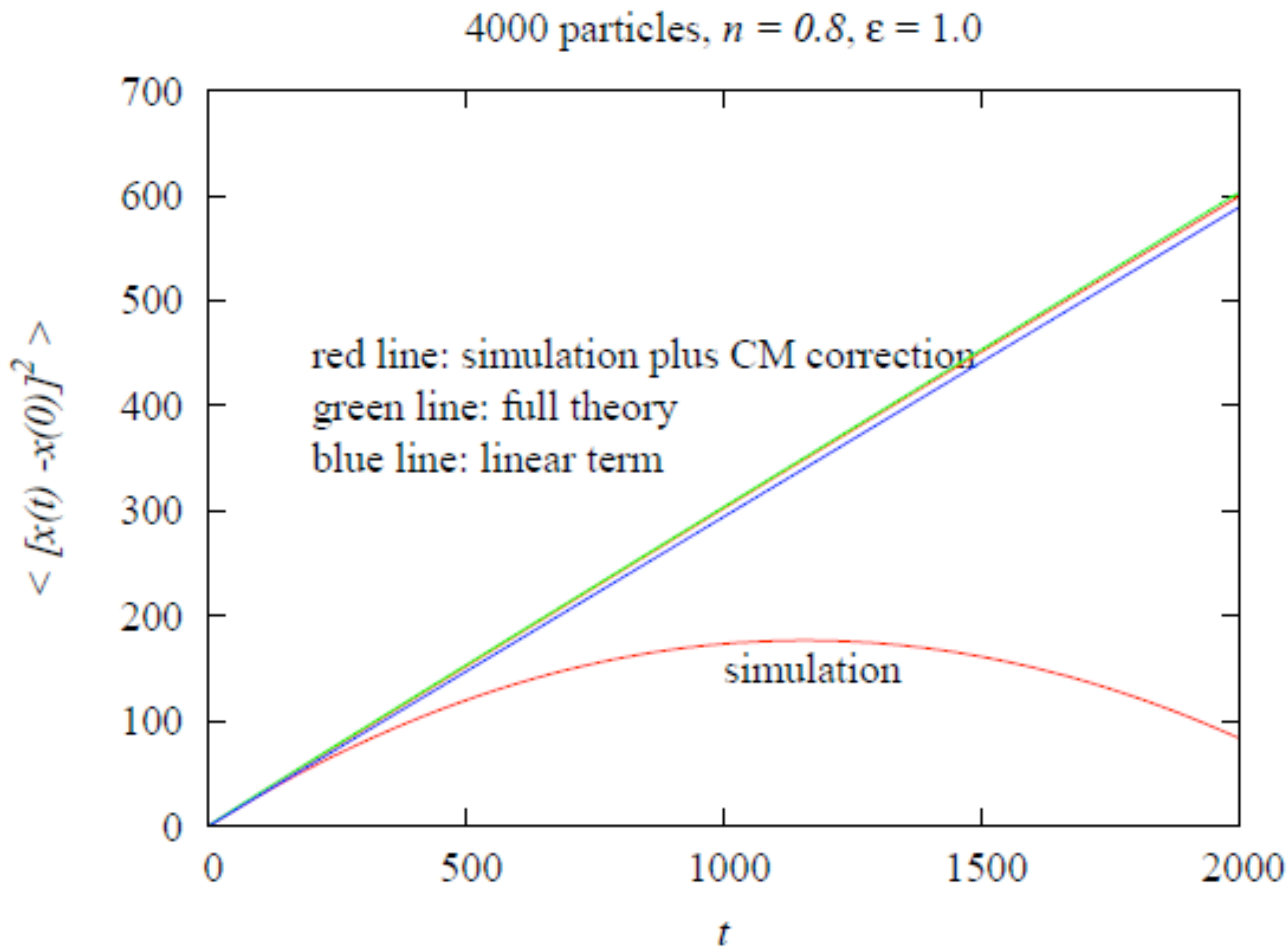

FIG. 7: Comparison of experimental and theoretical MSD for 4000 particles.

References on SFD:

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Conference on single file dynamics in Erice from July 4-9:

http://singlefiledynamicsconference.net/