Fluctuation theorem in colloidal systems with quenched disorder

Jeff Drocco

Princeton University

Krell Institute DOE CSGF Conference

June 17, 2008

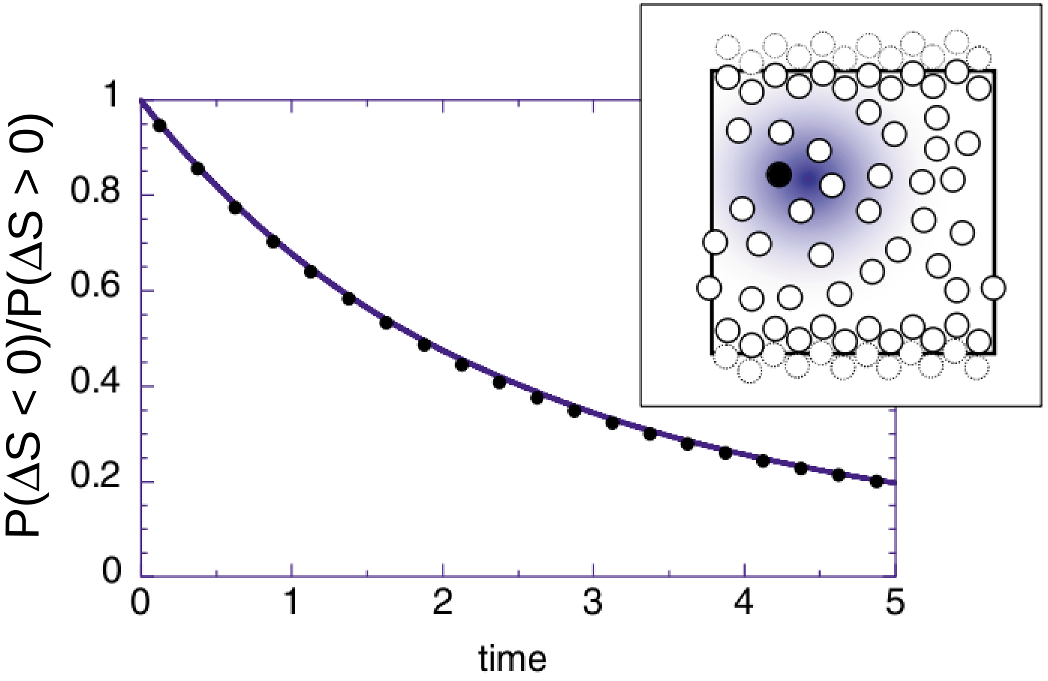
Second Law Violations

2^{nd} Law of Thermodynamics:

“The entropy of the universe tends to a maximum.” (Clausius)

“Experimental Demonstration of Violations of the Second Law of Thermodynamics for Small Systems and Short Time Scales”

G.M. Wang, et al., Phys. Rev. Lett. ***89****, 050601 (2002)*



Miniaturized devices do not behave like their larger counterparts!

Fluctuation Theorem

Evans, Cohen, Morriss: “Probability of Second Law Violations in Shearing Steady States” (1993)

- Quantifies the probability of short-term second law violations in a finite system
- Valid far from equilibrium

Compute average injected power over an interval τ

$$J_\tau(t) = \frac{1}{\tau}\int_t^{t+T} \vec{F}(t')\cdot\vec{v}(t')\,dt'$$

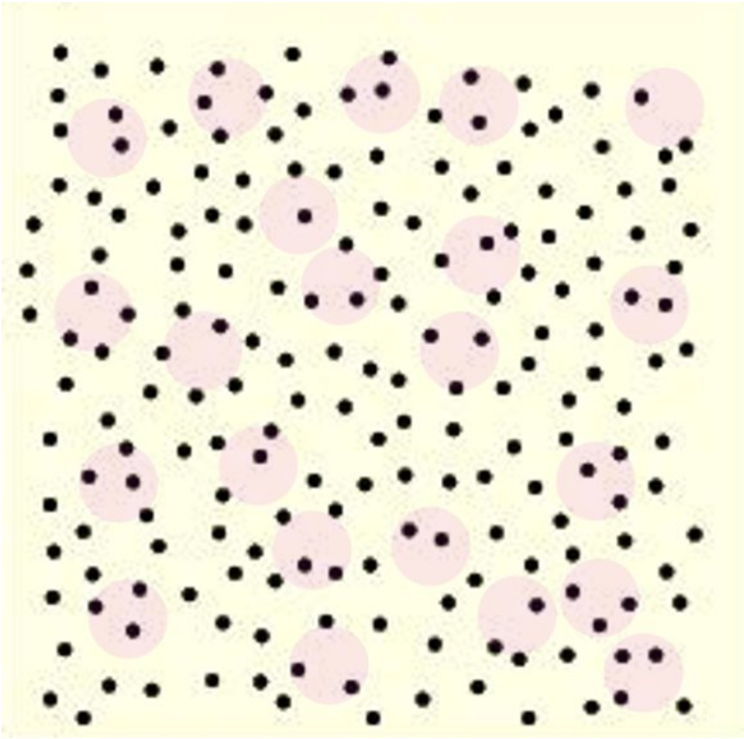
FT: The probability density function of J_τ follows

$$\frac{P(J_\tau=\epsilon)}{P(J_\tau=-\epsilon)} = e^{\beta\epsilon\tau} \qquad as\,\tau\to\infty$$

β^{-1} can be considered an “effective temperature”

Simulation parameters

- Screened Coulomb (Yukawa) interparticle interaction
- Quenched disorder simulated by randomly placed parabolic traps
- Overdamped dynamics; velocity Verlet integration



$$V(r_{ij}) = \frac{Q^2}{|\vec{r}_i - \vec{r}_j|} e^{-\kappa|\vec{r}_i - \vec{r}_j|}$$

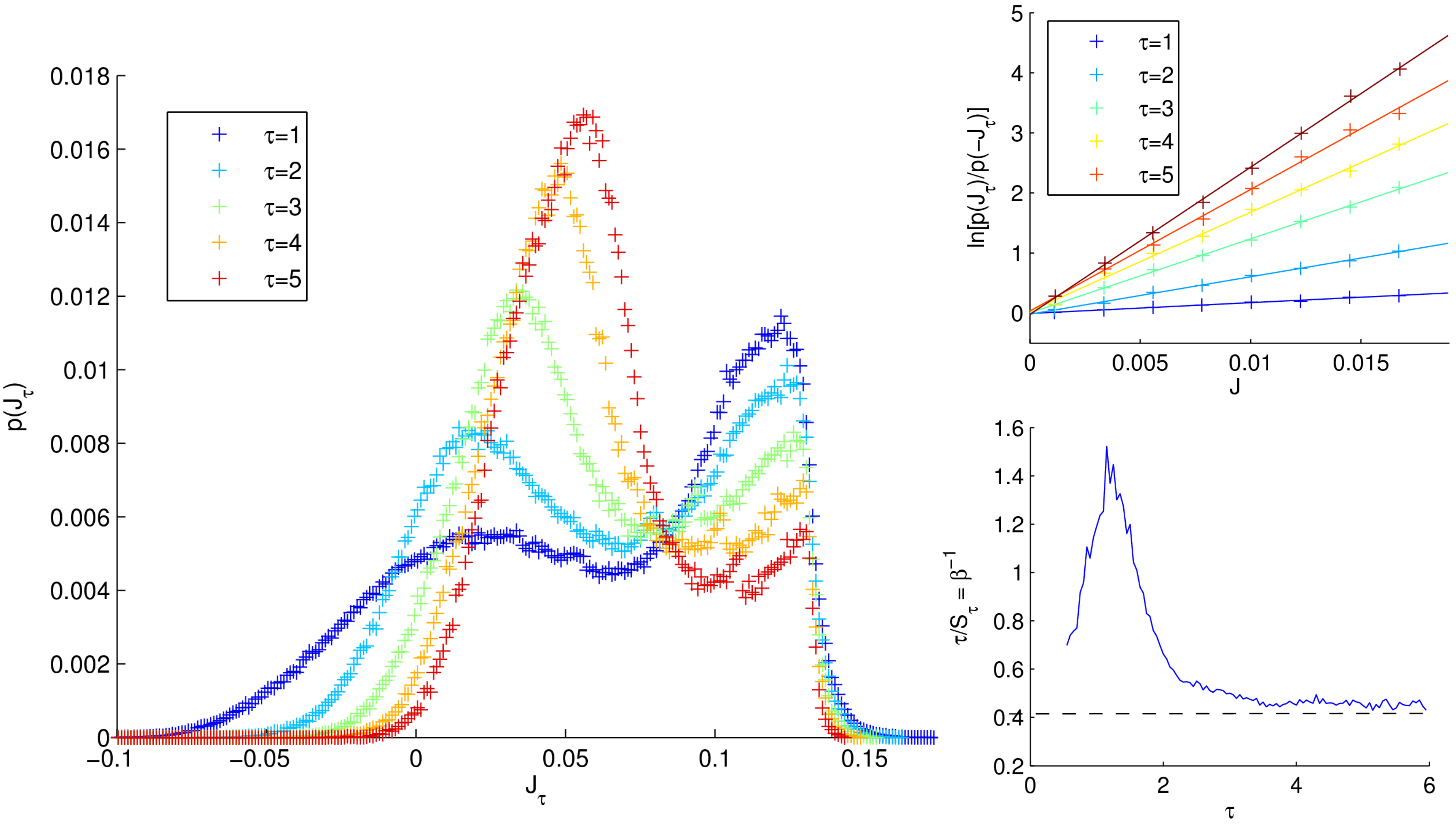
$$\frac{d\vec{r}_i}{dt} = \sum \vec{F}_{ij} + \vec{F}_p + \vec{F}_d$$

interparticle repulsion

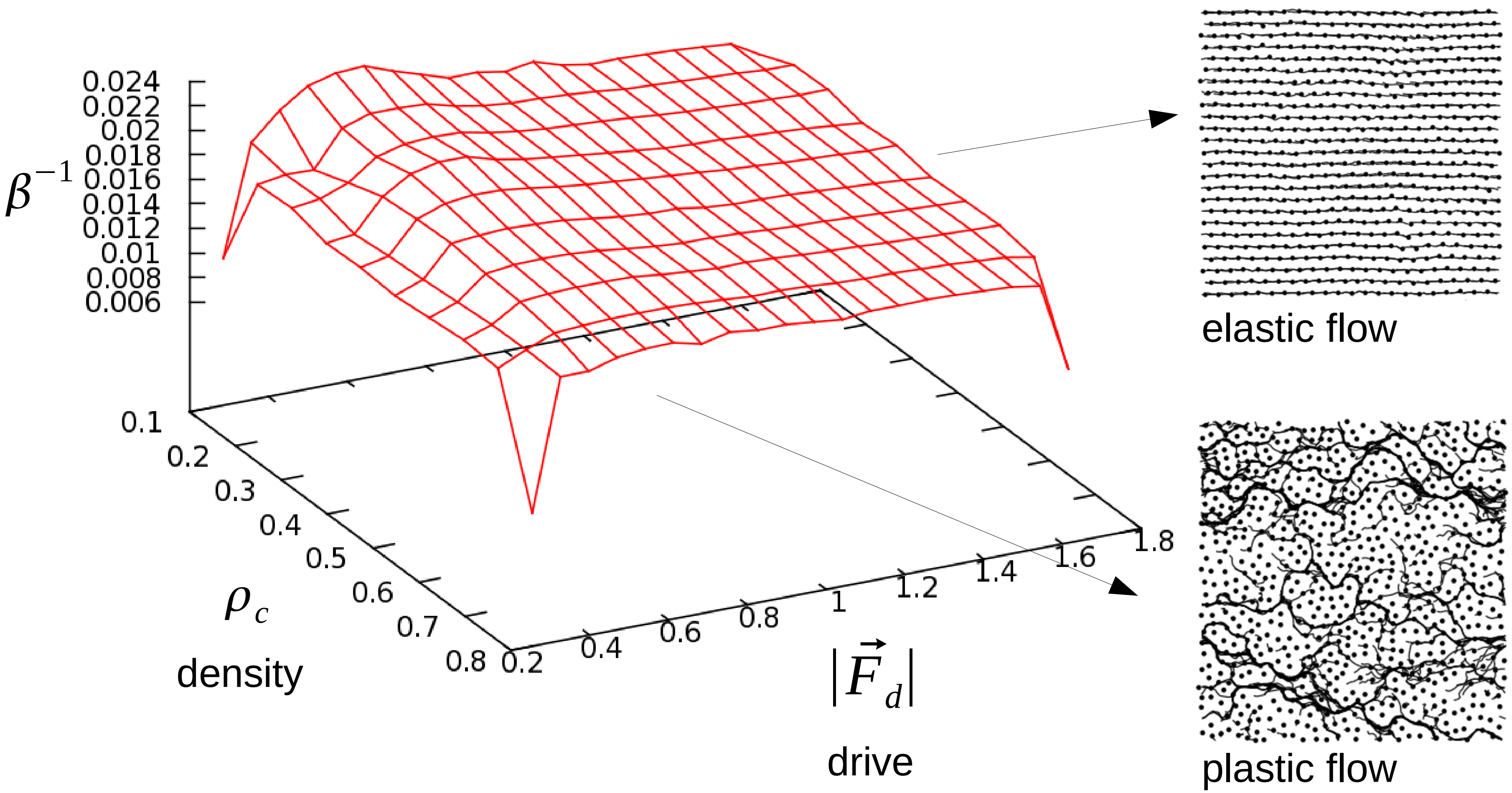
pinning force

drive

Probability Density Function

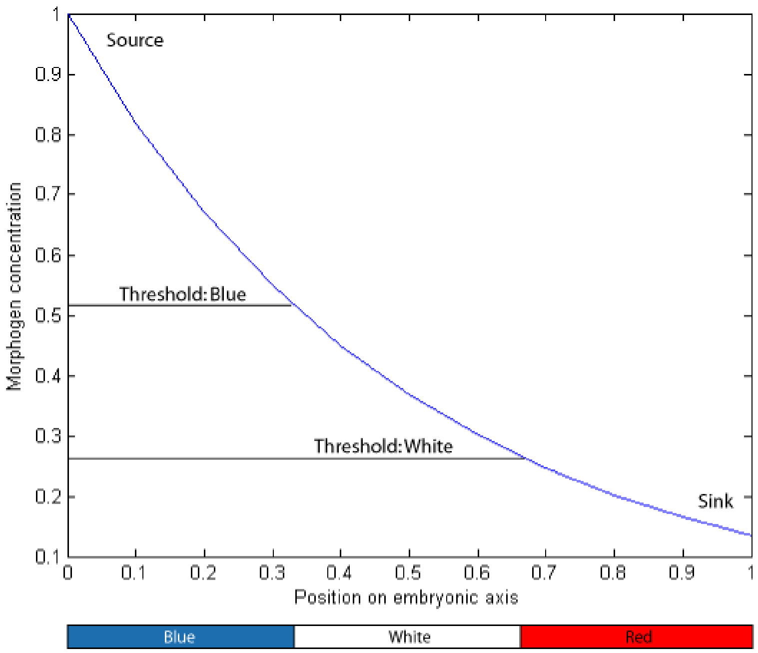


Effective Temperature

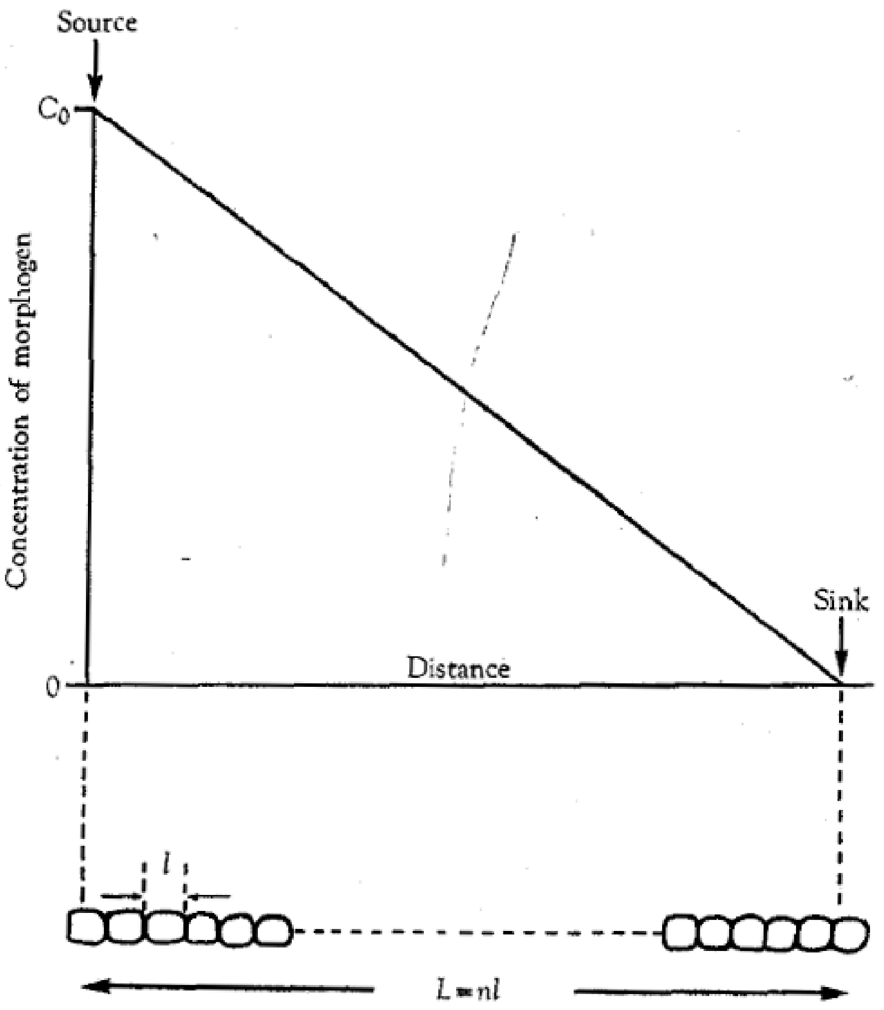


Diffusion in Biological Systems

Crick, 1970: Nature has difficulty evolving elaborate biochemical mechanisms. Diffusion is a likely candidate for establishing gradients.

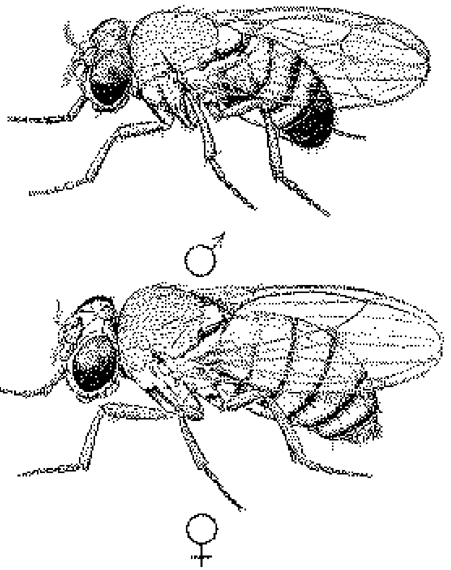


S.F. Gilbert, *Developmental Biology*, Sinauer



F. Crick, Nature ***225****, 421 (1970)*

Some Observed Gradients

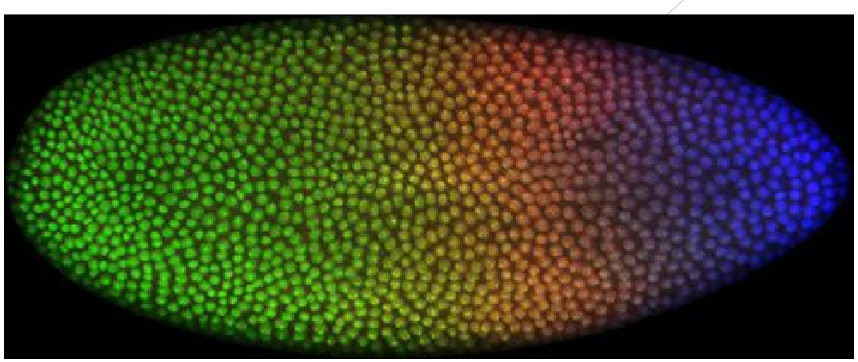


post.queensu.ca/~forsdyke/images/muller01.gif

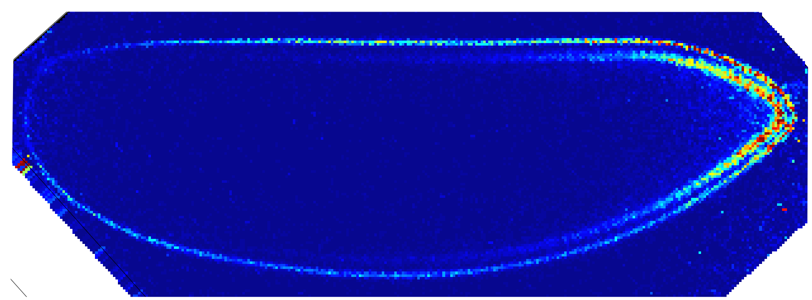
- *D. melanogaster* (fruit fly)

http://www.bio.brandeis.edu/weltelab/images/embryopic.gif

FlyEx database, Reinitz lab, SUNY-Stony Brook

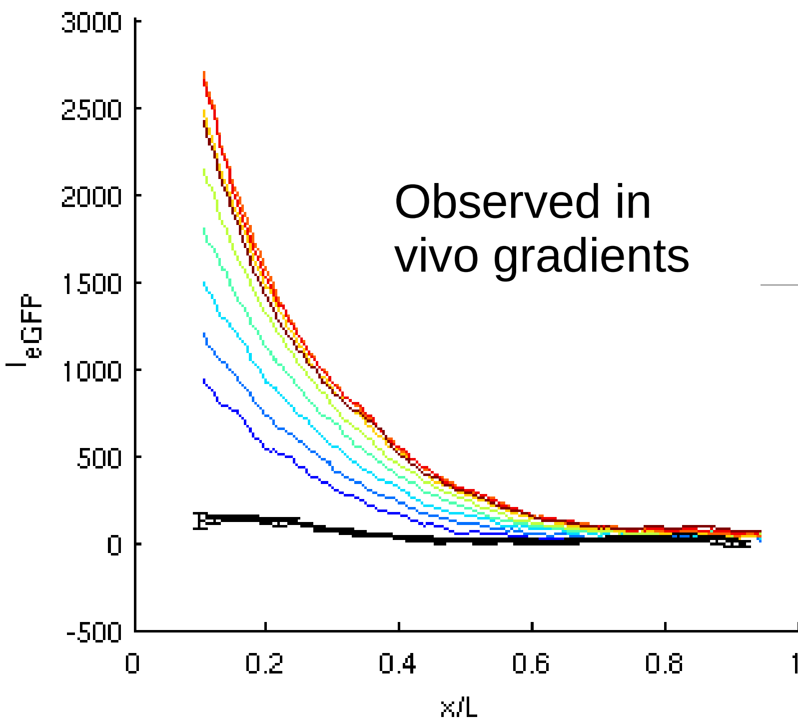


Caudal – Even-skipped -- Bicoid

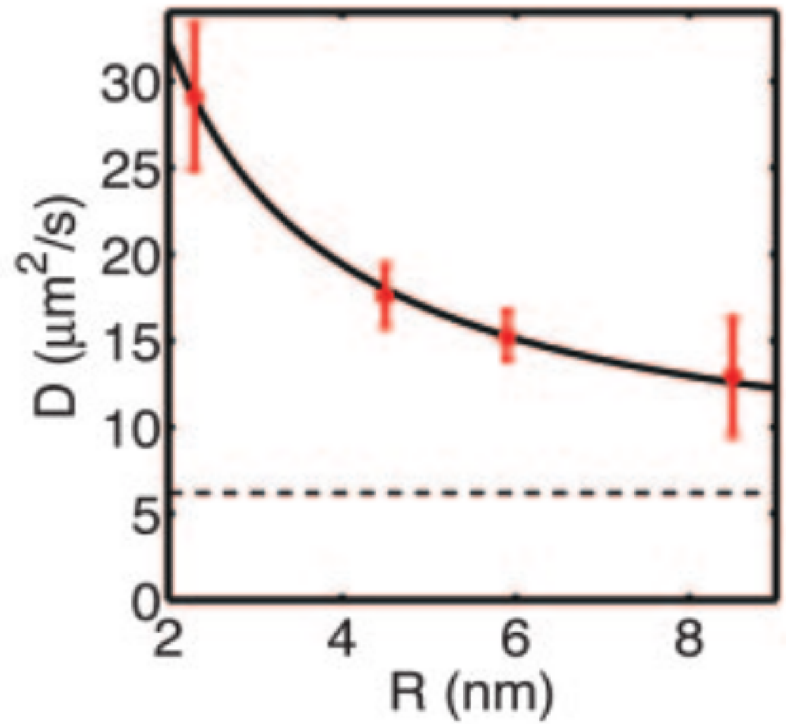


Bicoid *in vivo*

Problems with the Crick model



T. Gregor et al., PNAS ***102***, *18403 (2005)*

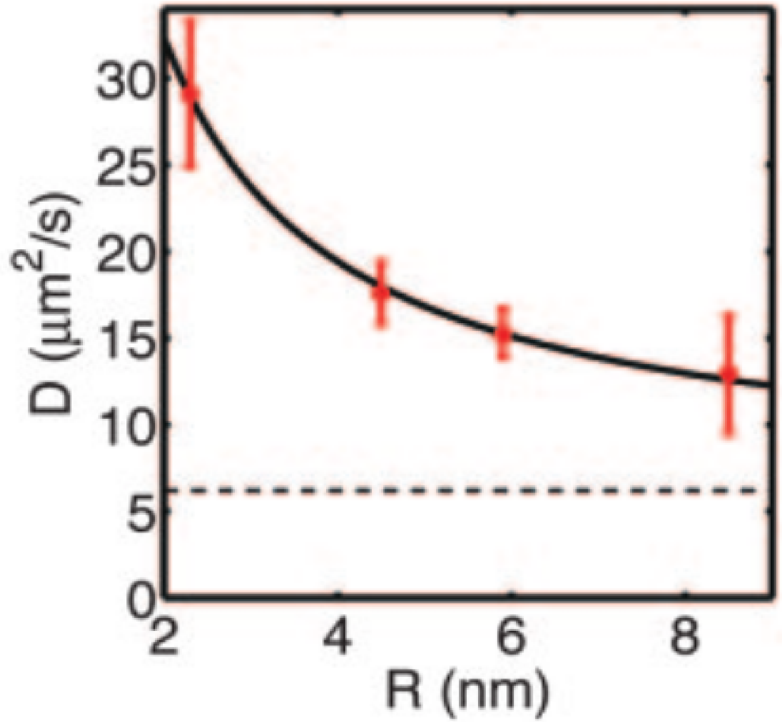


Stokes' radius

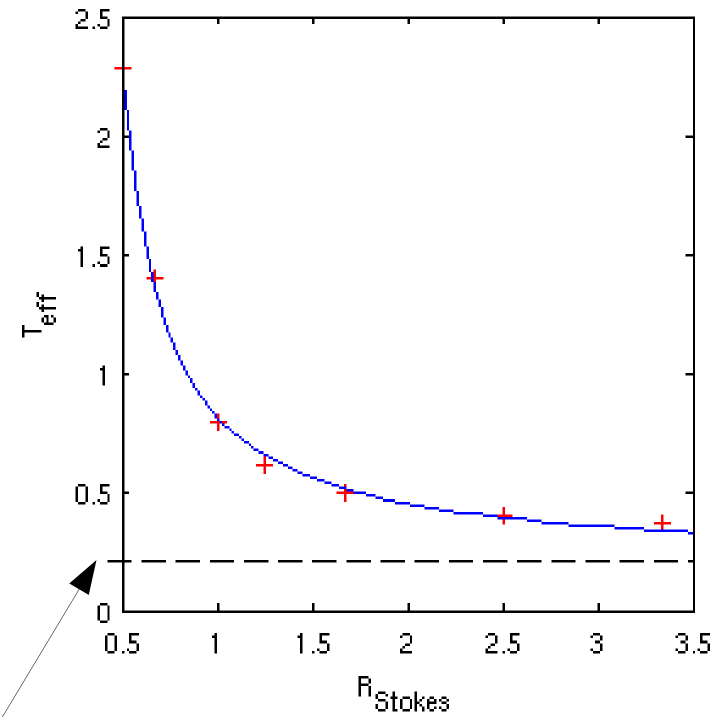
Stokes-Einstein relation: $D = \frac{k_B T}{6 \pi \eta r}$ + C stirring?

Analog with effective temperature

T. Gregor et al., PNAS ***102***, *18403 (2005)*



Stokes' radius



additive non-thermal offset

Summary

- We verify that colloidal particles dragged over a disordered substrate with constant applied drive have probability density functions of injected power corresponding to predictions of the fluctuation theorem.

- An “effective temperature” can be defined in both the plastic and elastic flow regimes despite the fact that the colloid is a dissipative, non-equilibrium system.

- Quenched disorder should be considered as a model in explaining transport behavior of biological molecules.

Acknowledgements

Princeton

- David Tank, Physics & Mol. Bio.
- Eric Wieschaus, Mol. Bio.
- Bill Bialek, Physics
- Oliver Grimm
- Thomas Gregor
- Stefan Thiberge

LANL

- Cynthia Olson-Reichhardt, T-12
- Charles Reichhardt, T-13

- Krell Institute, Computational Science Graduate Fellowship
- Department of Energy
- National Institutes of Health
- Howard Hughes Medical Institute