Dynamical phase transitions and facilitation in a glass former model

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Faculty Fellow, New York University

Soft Condensed Matter Center Group Meeting
September 19th, 2011

I couldn't have done this without...

September 29, 2011 Thursday 4:00 PM
Meyer 122
Physics Colloquia (colloquia)

David Chandler
University of California, Berkeley

The Glass Transition: Order-disorder in Trajectory Space

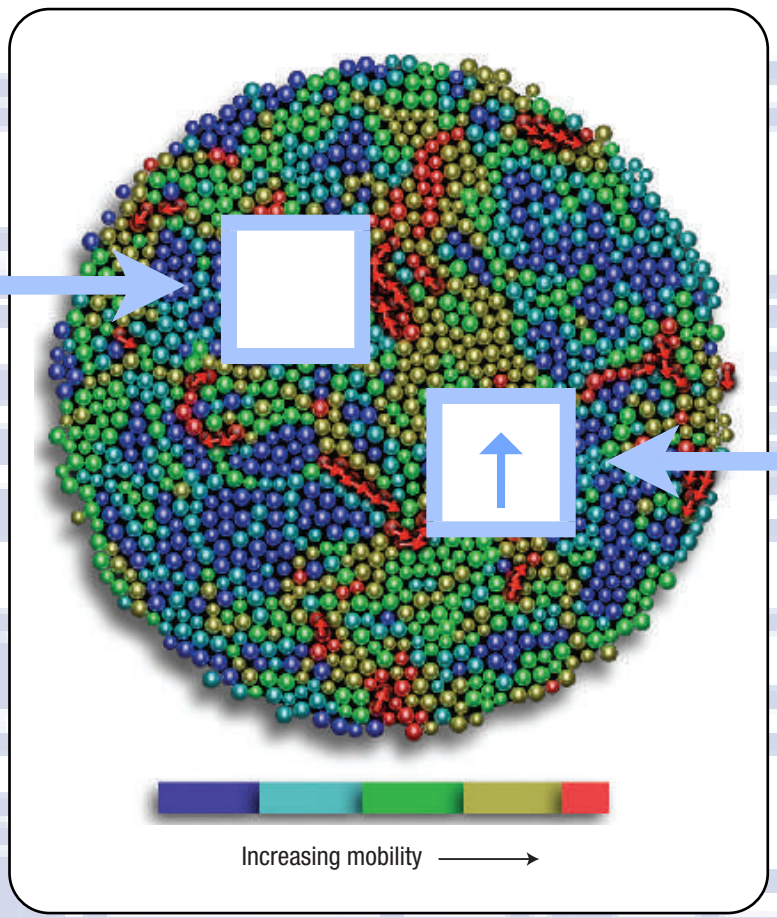
A picture is drawn of viscous liquid dynamics on the way to forming glass. Excitations are directional and localized in space and time, and relaxation proceeds through hierarchical dynamics, with excitations facilitating the the birth and death of neighboring excitations. Reversible dynamics and thermodynamics in glass forming liquids are non-singular, and transport properties are characterized by simple scaling relationships. In contrast, out of equilibrium there is an order-disorder transition between the liquid and a glass. Dynamic heterogeneity in equilibrated structural glass formers is a pre-wetting associated with this non-equilibrium phase transition.

The Chandler Group, Fall 2010

Robert L. Jack

Motivation: dynamic facilitation

Mostly Immobile (Unexcited) Particles



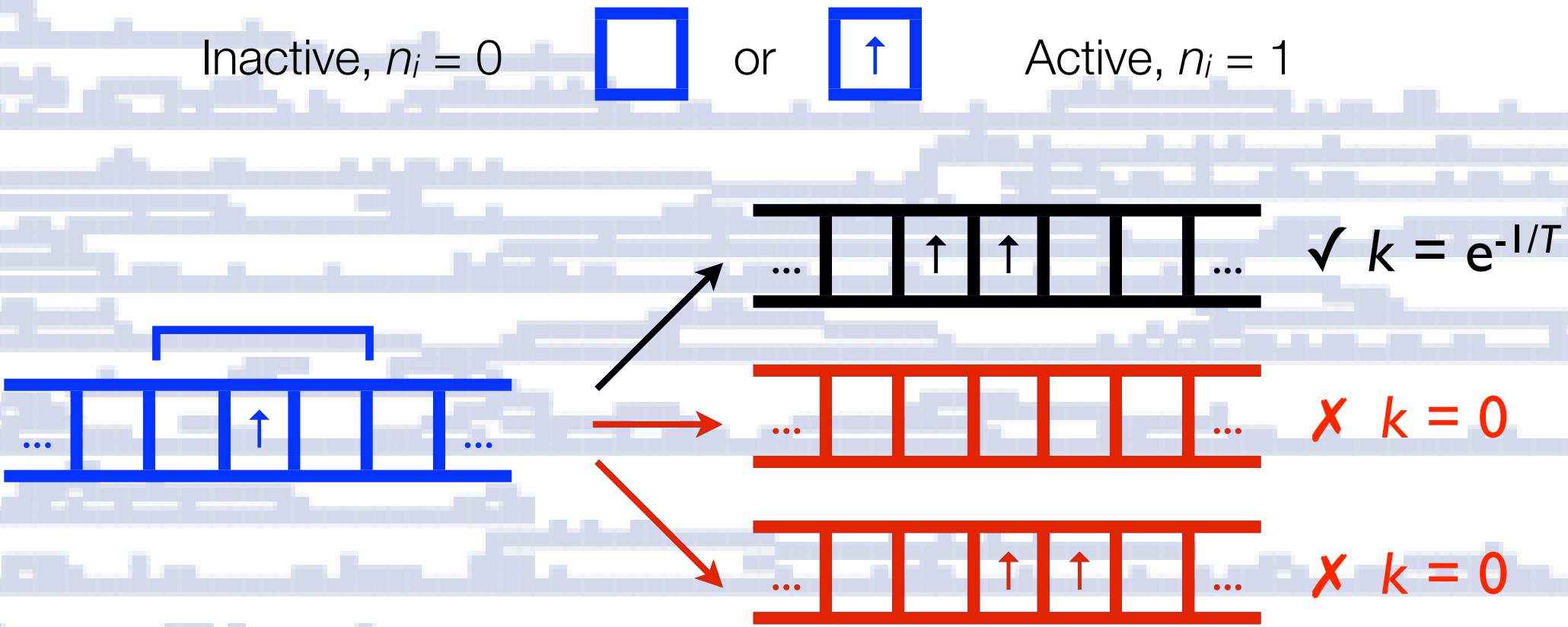
Mostly Mobile (Excited) Particles

AS Keys, AR Abate, SC Glotzer, DJ Durian. *Nature Physics*. **3**, 260-264 (2007).

The kinetically constrained east model

Noninteracting lattice gas with N sites and kinetic constraints.

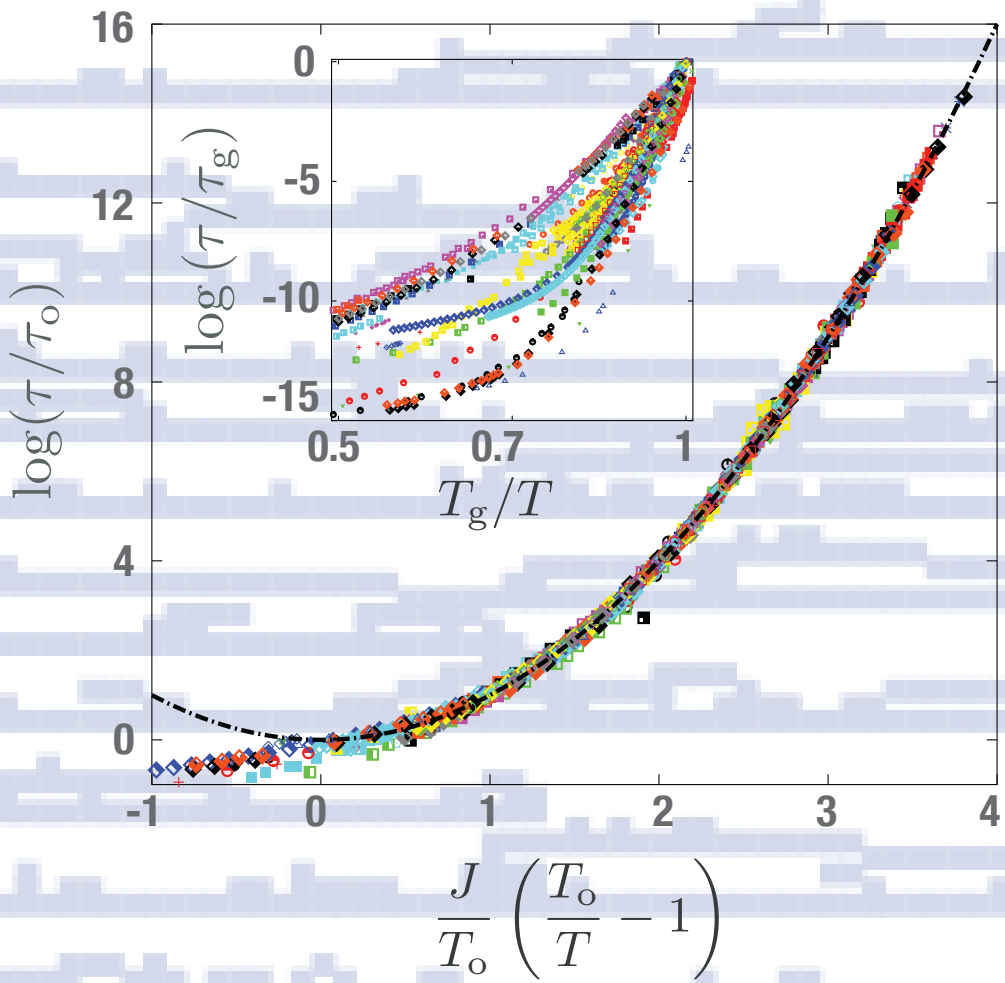
Sites can take on two values:

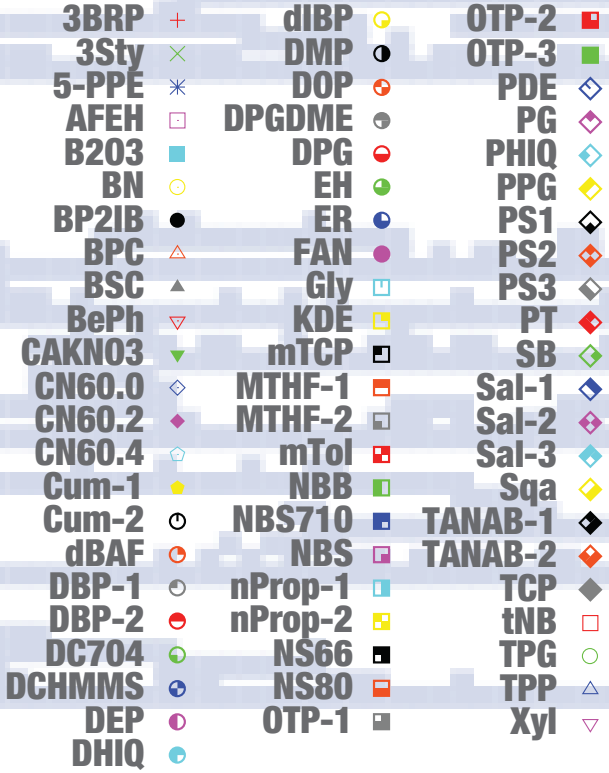


S. Eisinger and J. Jackle, *Z. Phys. B Condens. Matter*. **84**, 115–124 (1991).

Why is the east model a good fragile glass former model?

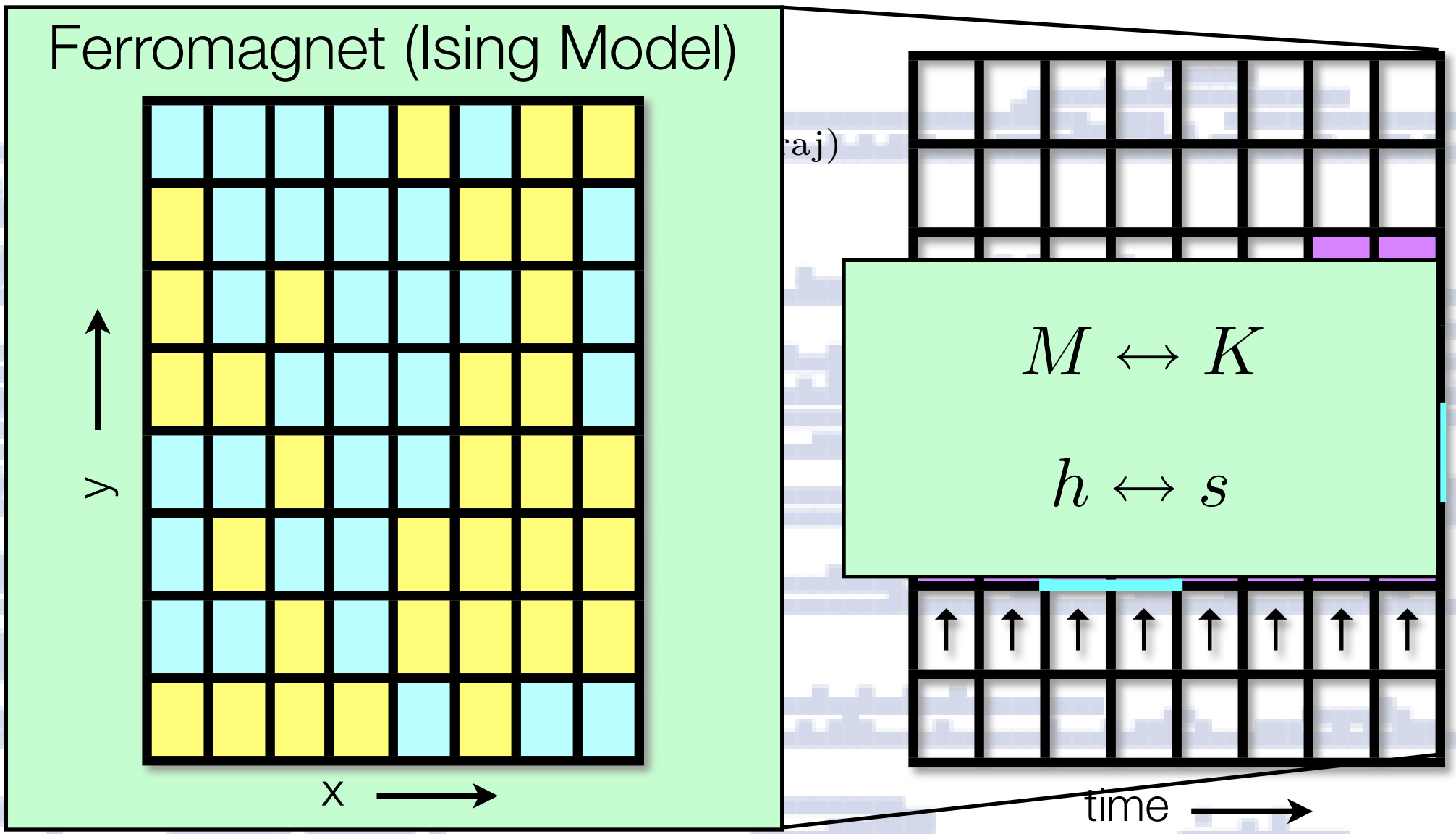
Based on this model we can derive a form[1,2] that collapses data for fragile glassformers:





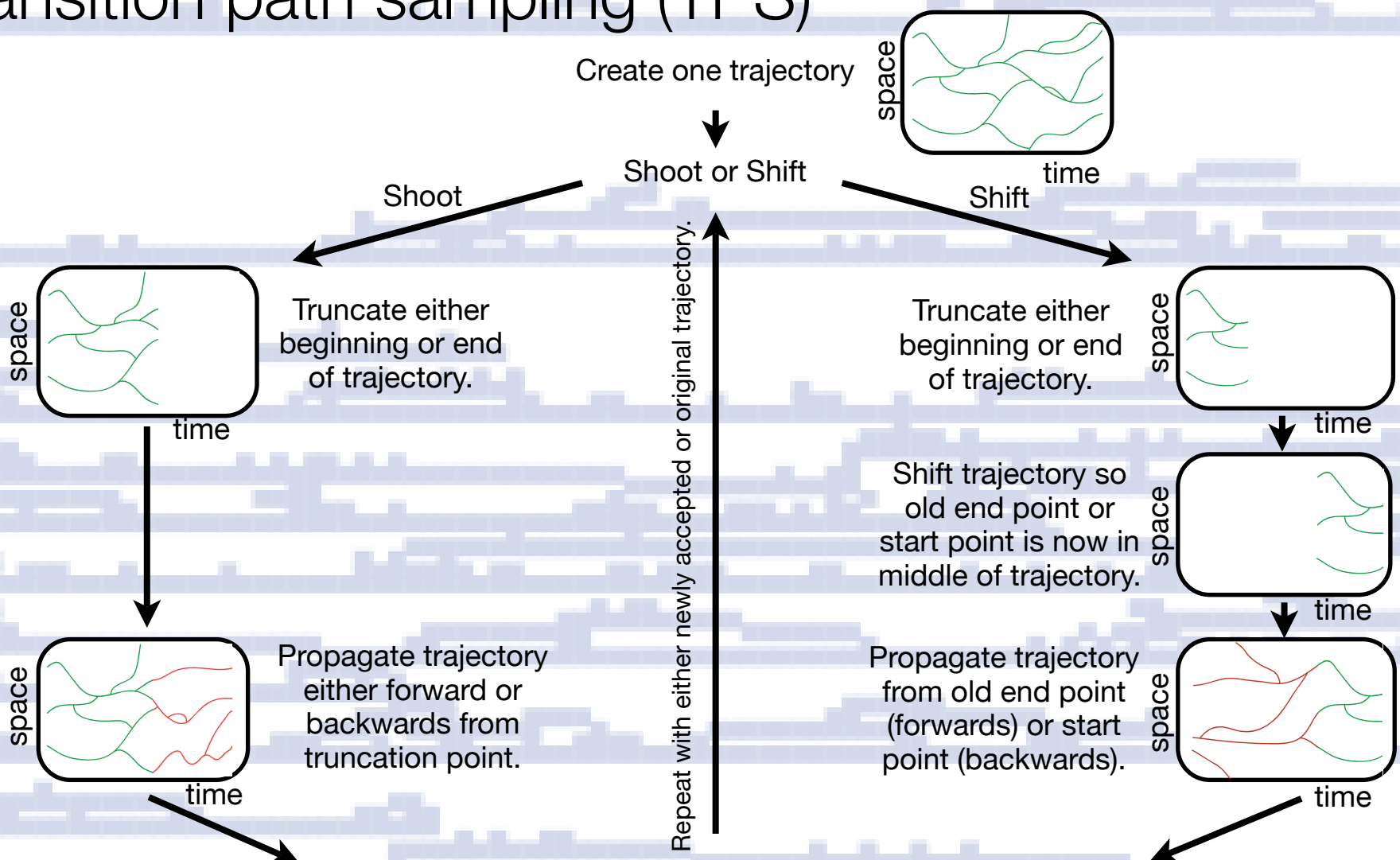
[1] J. P. Garrahan and D. Chandler, *Proc. Natl Acad. Sci.* **100**, 9710-9714 (2003).
[2] Y. S. Elmatad, J. P. Garrahan, D. Chandler. *J. Phys. Chem. B*. **113**, 5563 (2009).

Ensembles of trajectories: Biasing in the *s*-ensemble



[1] Y. S. Elmatad, R. L. Jack, J. P. Garrahan, D. Chandler. *Proc. Natl. Acad. Sci*. **107**, 12793 (2010).

Transition path sampling (TPS)



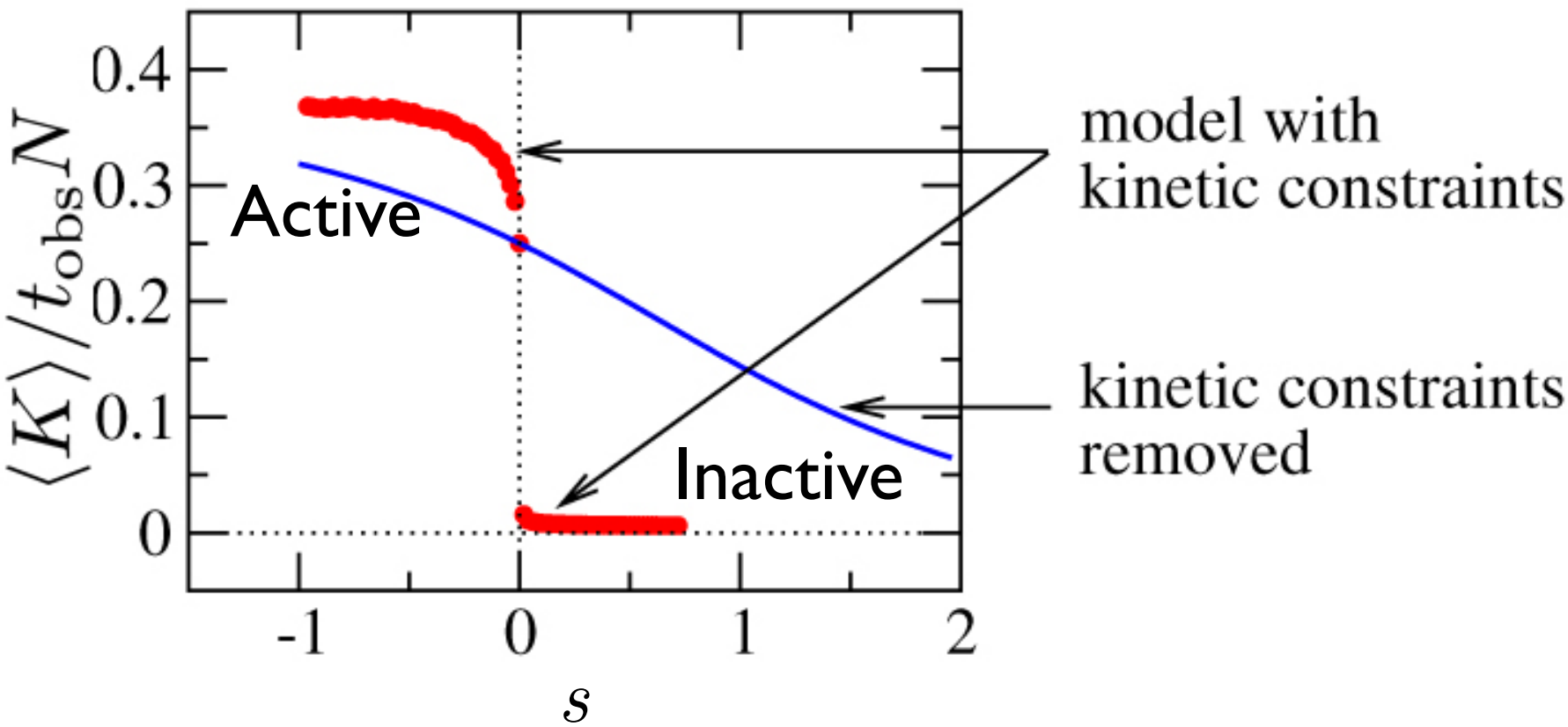
$$\text{Accept with } P = \min\left\{1, e^{-s\Delta K(\text{traj})}\right\}$$

$$\Delta K = K(\text{new traj}) - K(\text{old traj})$$

If accepted, replace old trajectory with new trajectory

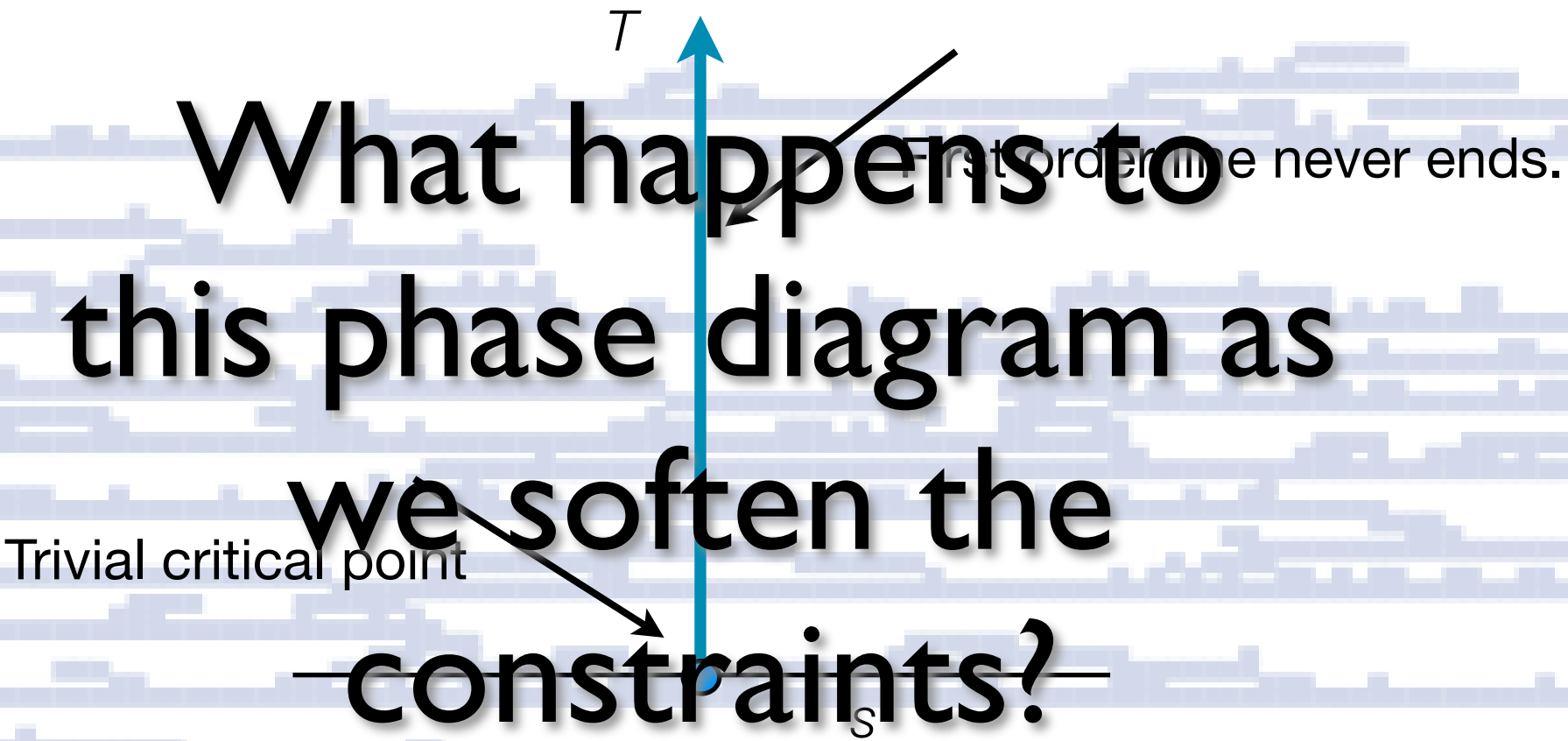
P.G. Bolhuis, D. Chandler, C. Dellago, & P.L. Geissler. *Annu. Rev. Phys Chem.* 2002 53:291-318.000

First order phase transition in east model



J. P. Garrahan, R. L. Jack,V. Lecomte, E. Pitard, K. van Duijvendijk and F. van Wijland, *Phys. Rev. Lett.* 98, 195702 (2007).

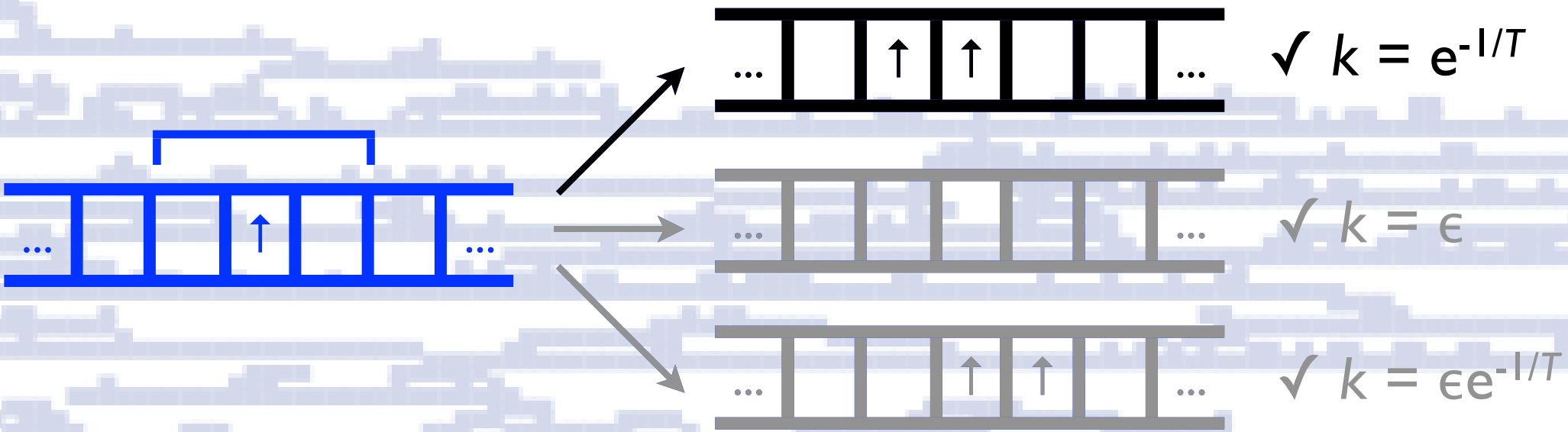
East model phase diagram



What happens to this phase diagram as we soften the constraints?

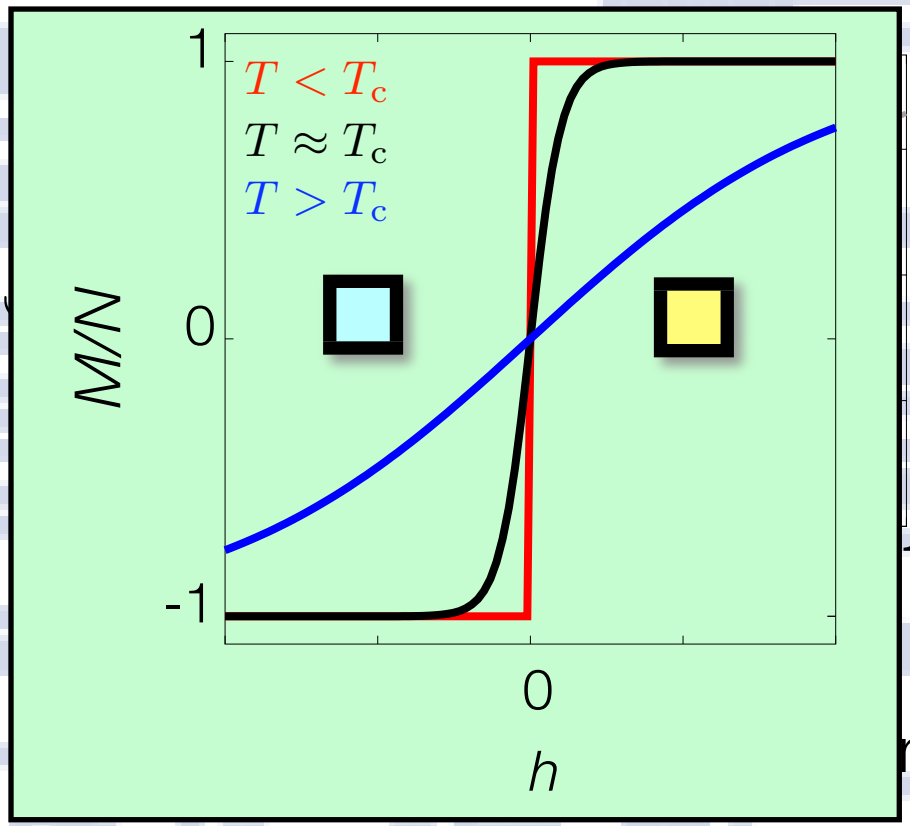
J. P. Garrahan, R. L. Jack,V. Lecomte, E. Pitard, K. van Duijvendijk and F. van Wijland, *Phys. Rev. Lett.* 98, 195702 (2007).

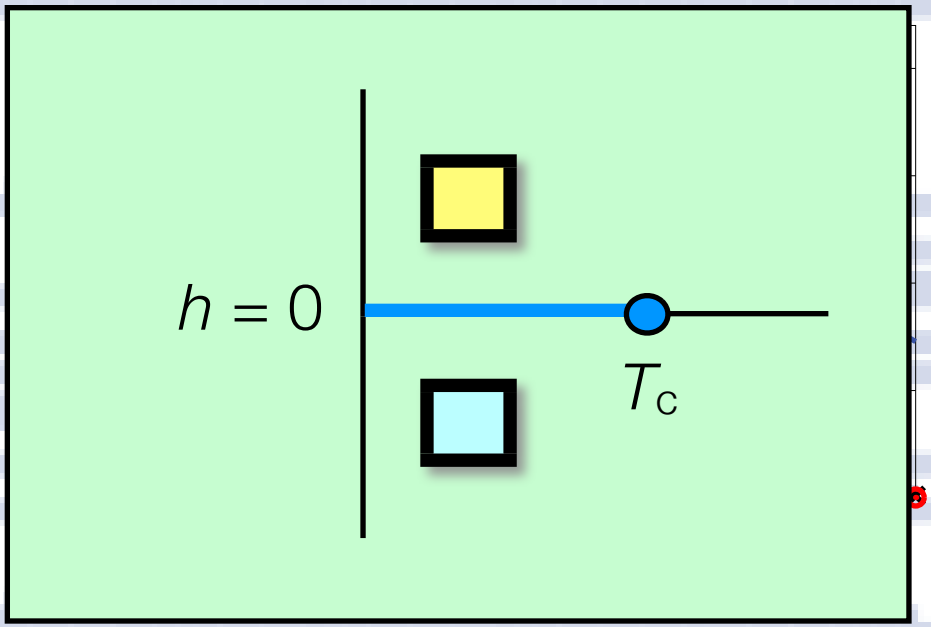
The *soft* east model



Phase diagram shows critical point

$$k = K/t_{\mathrm{obs}}N$$





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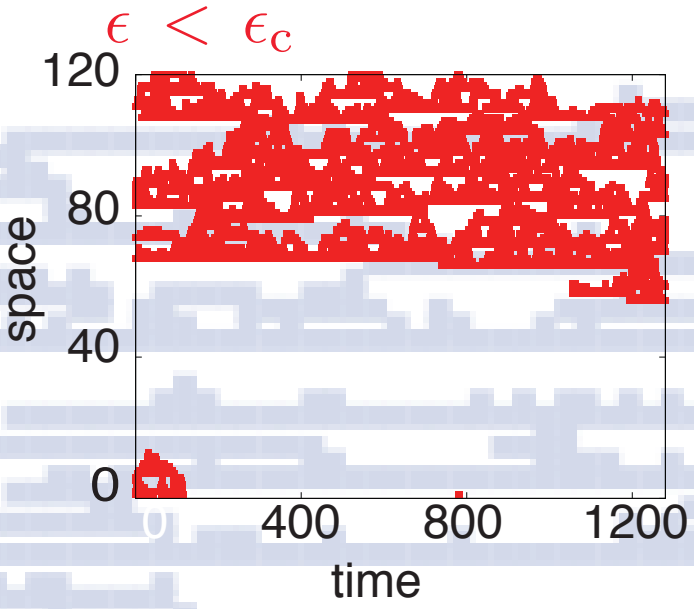
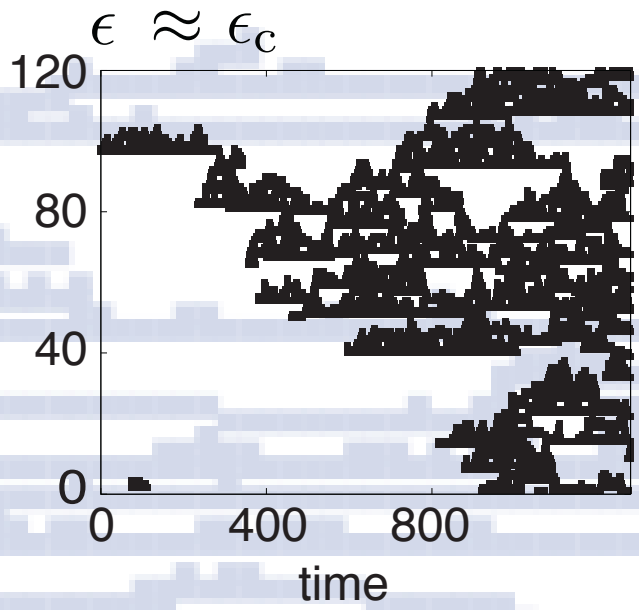
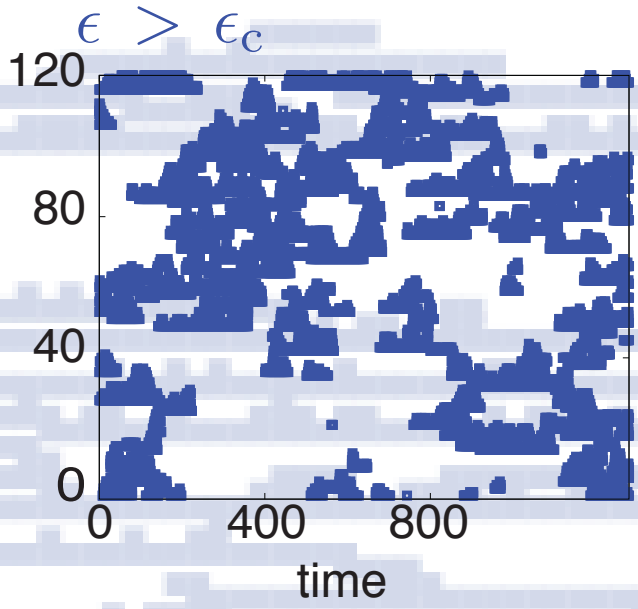
$\epsilon < \epsilon_C$ is the first order phase transition region.

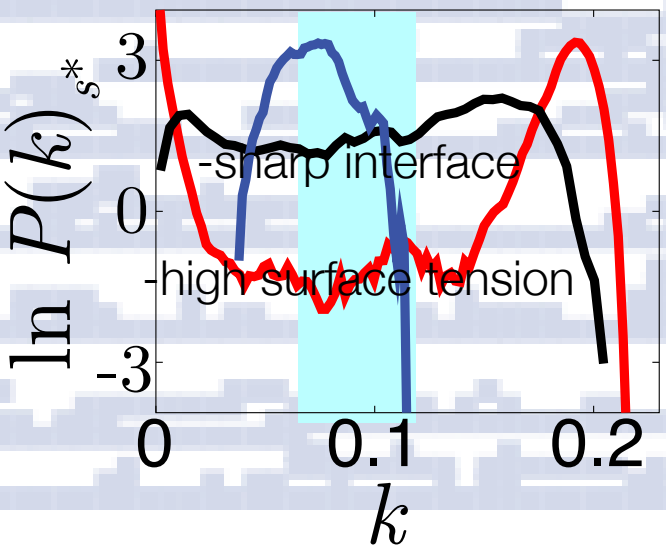
$\epsilon > \epsilon_C$ is the one phase region.

Sample trajectories from transition region









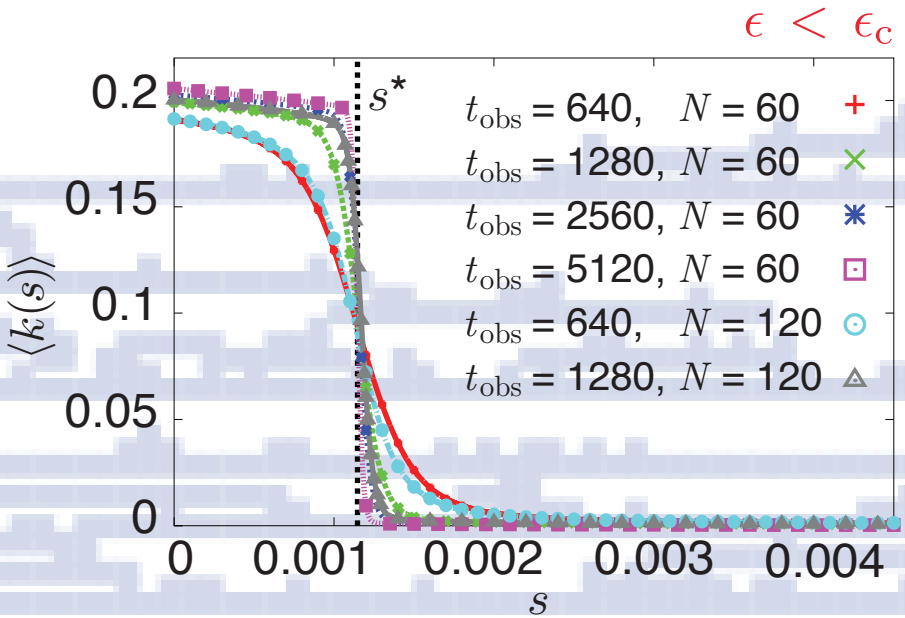
-amorphous interface

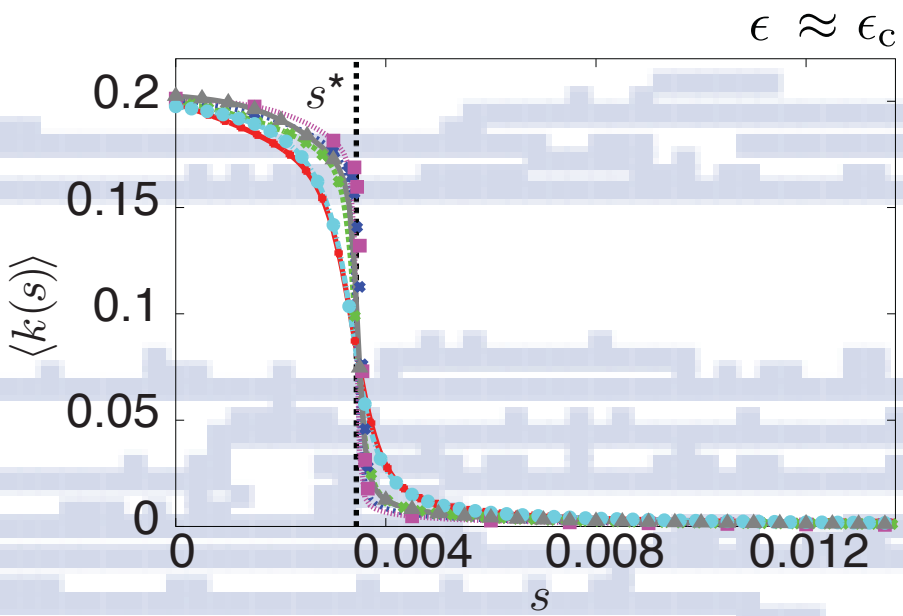
-low surface tension

-system spanning clusters

-one phase

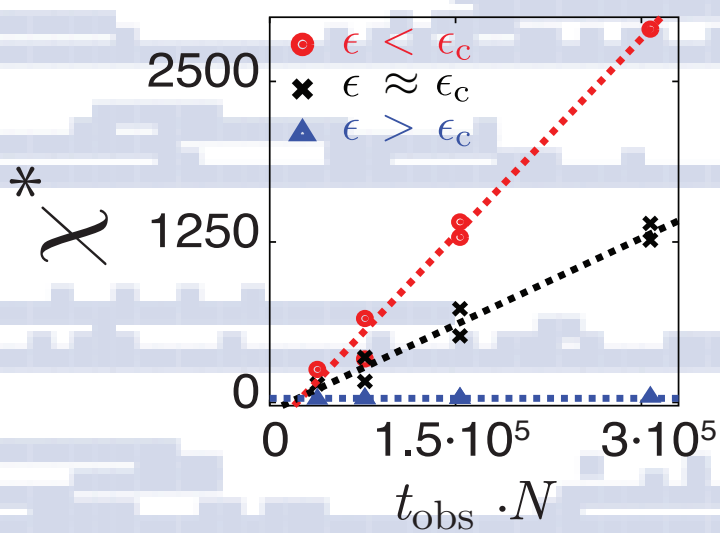
Finite size scaling confirms transition



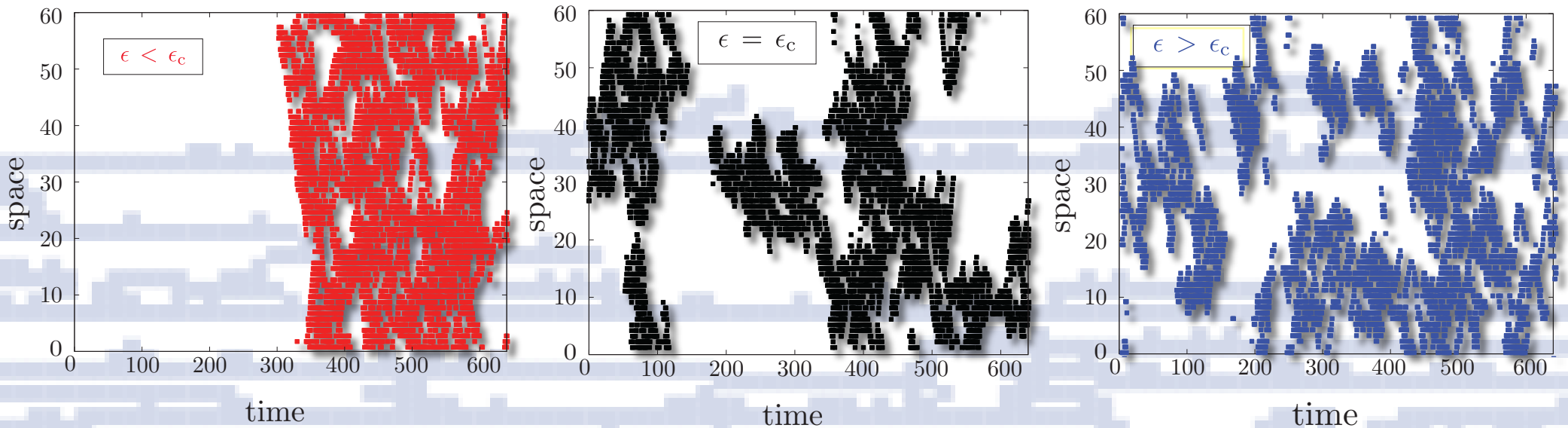


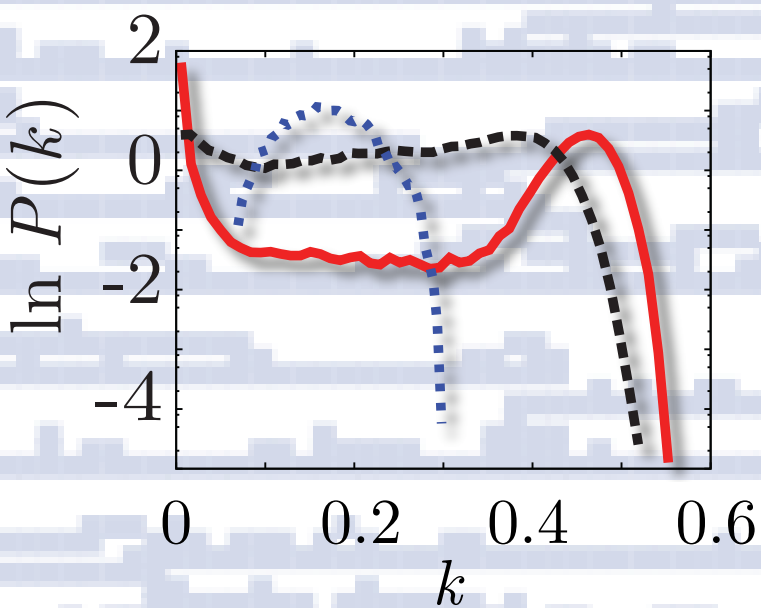
For a 1st order phase transition:

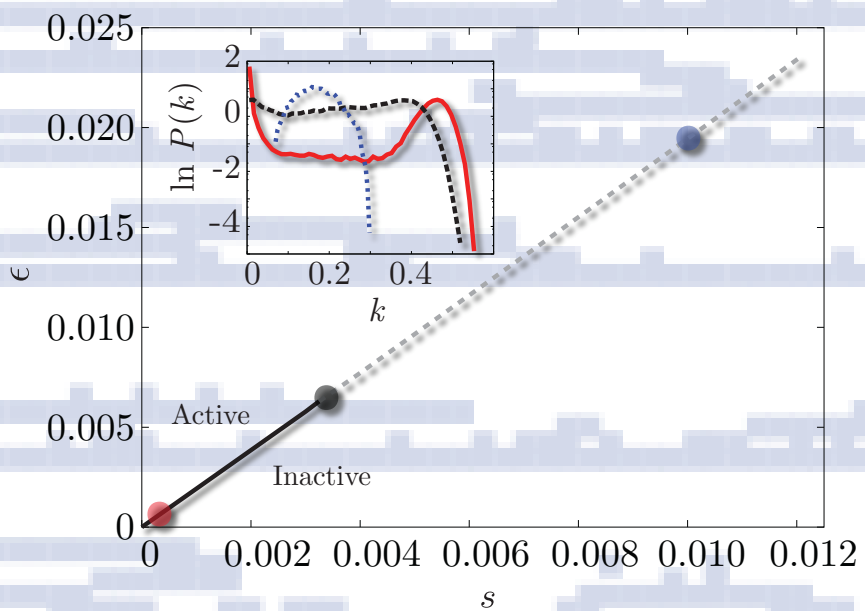
$$\chi^* = -\frac{d\langle k \rangle}{ds} \propto t_{obs} \cdot N$$



Other models: Fredrickson-Andersen mmodel







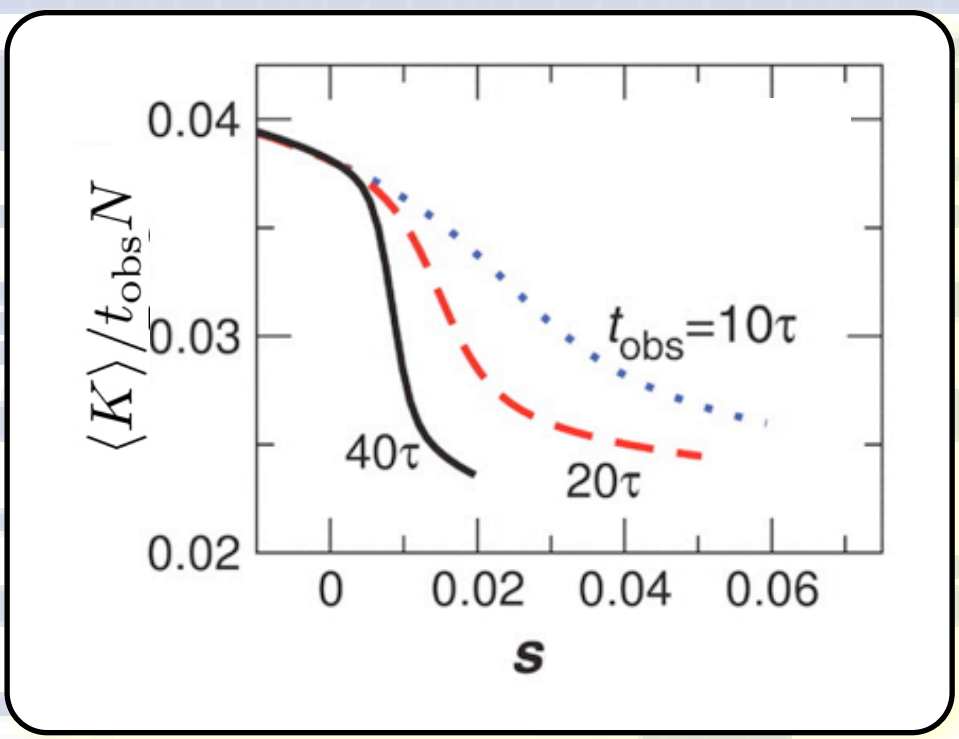
Y. S. Elmatad, R.L. Jack, D. Chandler, and J.P. Garrahan. *Proc. Natl. Acad. Sci.* **107**, 12793-12798, 2010.

What about atomistic systems?

Binary mixture of small and large Lennard-Jones Particles

Analogous order parameter in continuous space:

$$K[\mathrm{traj}] = \Delta t \sum_{t=0}^{t_{\mathrm{obs}}} \sum_{j=0}^{N} |r_j(t+\Delta t) - r_j(t)|^2$$



Hedges, L.O, Jack, R. L, Garrahan, J.P, Chandler, D. Science, 323, 1309 (2009)

What does this have to do with “real” glasses?

Softening constraints on a 1d East model introduces a space-time critical point.

Finite size scaling confirms 2 phase, critical, and 1 phase regions.

Trajectories for $\epsilon < \epsilon_c$ show sharp, minimized interface.

For $\epsilon \approx \epsilon_c$ the interface is amorphous and system spanning.

For $\epsilon > \epsilon_c$ there is only one phase in accordance with expected behavior beyond a critical point.

An avoided space-time critical point may be an underlying cause of the glass transition for glass formers.