Avalanche dynamics

in a 2D glass

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Outline

- *Introduction (what is the question?)*
- *Equilbrium liquid (basic chracterization)*
- *Avalanche in glass at zero applied strain*
- *Summary and future plans*

Introduction

What is avalanche?

In response to a driving force -

- ***Collective displacement of a group of particles (loss of stability)***
- ***Sudden (intermittent dynamics)***
- ***Very common in nature (e.g. snow avalanche, earthquake)***

Introducion

Connection to glassy dynamics

***"Glass"* = system below T_g (*falls out of equilibrium on observation time scale*)**

Glass (non-equilibrium)	Supercooled liquids (equlibrium)
Aging	Structural relaxation
De-vitrification	Crystallization

Avalanche is relevant for aging and de-vitrification

Introduction

What is the driving force?

***Zero applied strain / stress* -**

Structure becomes more homogeneous by spontaneous thermal fluctuation

System tries to lower free energy

Externally applied strain / stress
(the above factors should still be relevant)

Response of the system

Loss of mechanical stability

Re-wiring of the force network

Problem : details

- **Polydisperse WCA model in 2D**

  Weakly frustrated against crystallization

  ψ_6 is a good order parameter.

- **Equilibrate (normal liquid)**

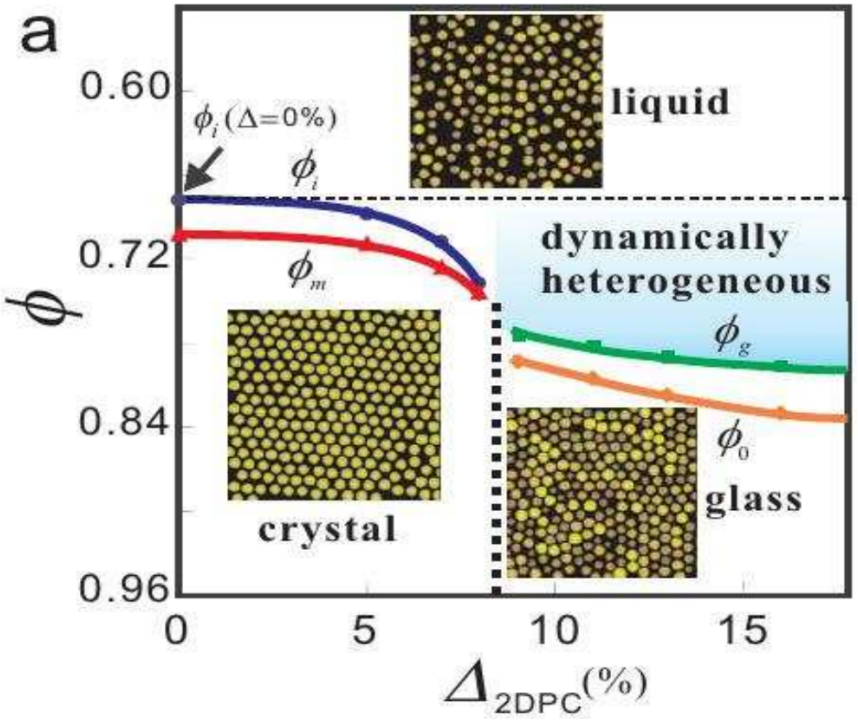
- **Quench and age at zero strain**

- **Apply shear**

- **Analyze real space events (re-wiring of force networks)**

- **Find "selection rules under shear" (where does it start, how does it propagate, why does it stop)**

Equilibrium Simulation details

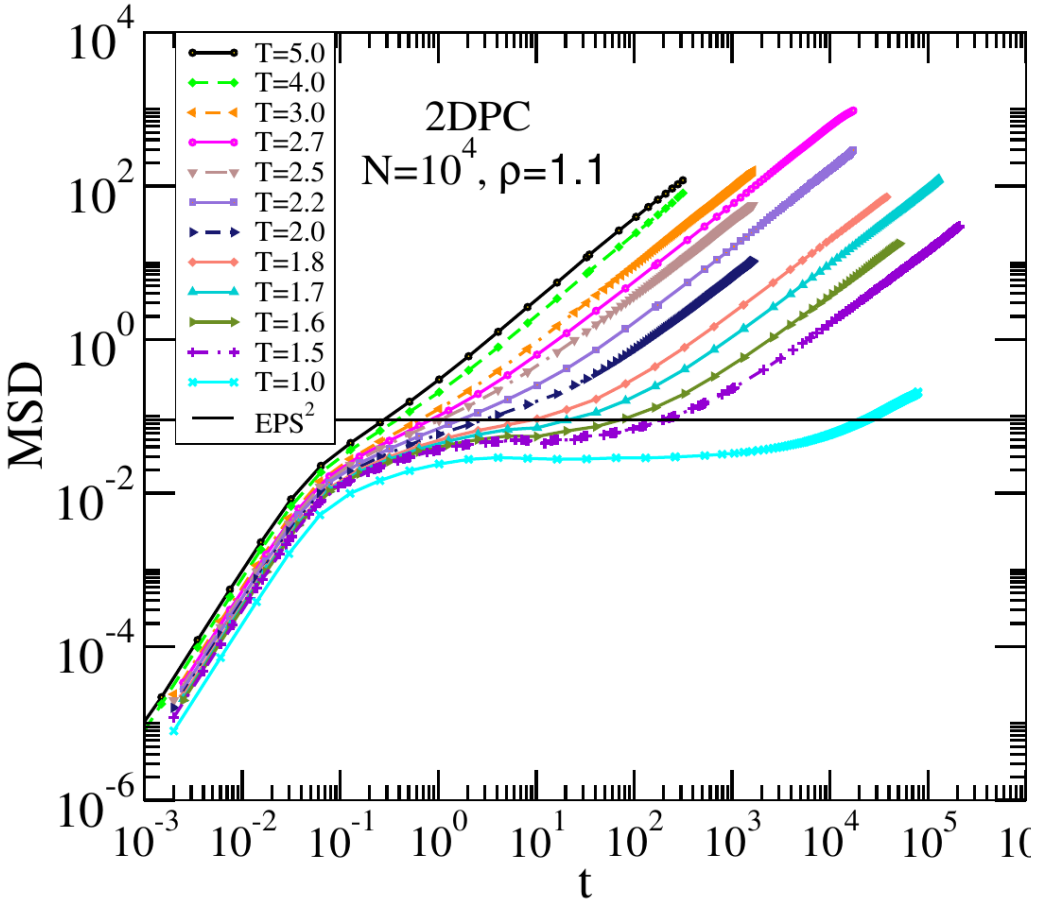


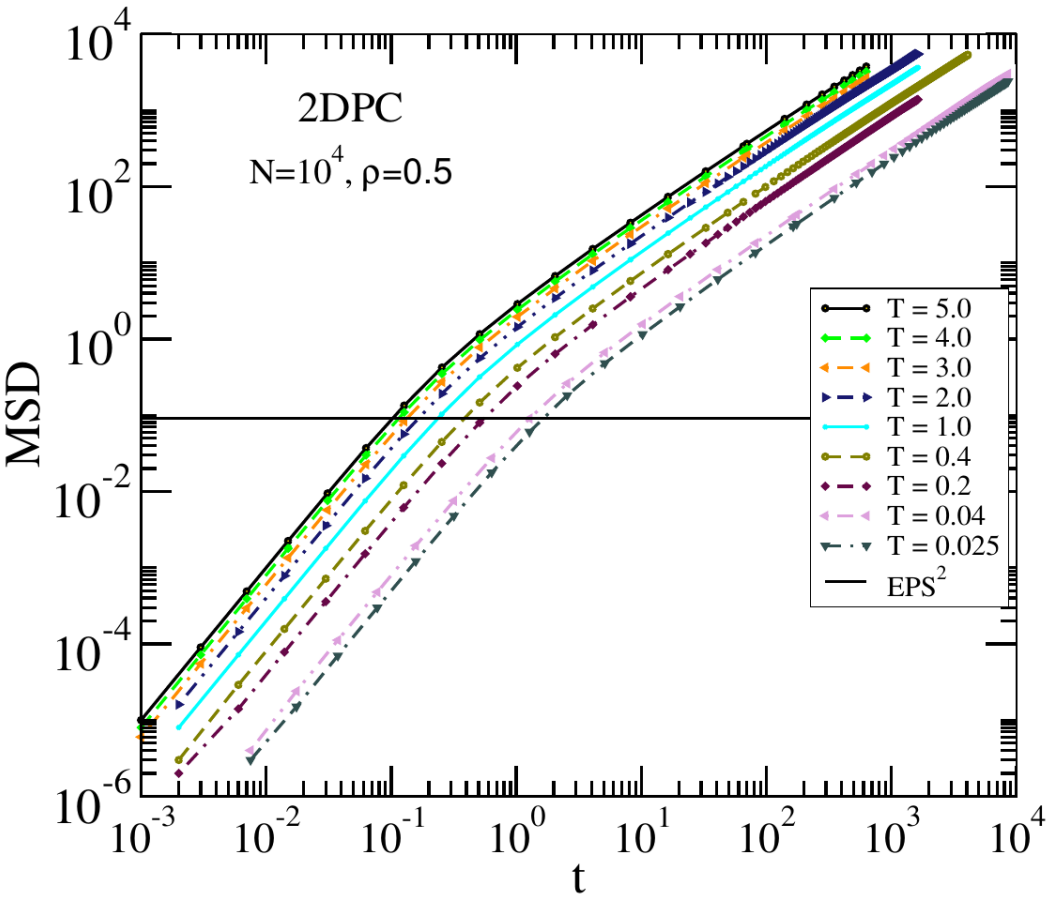
Quantity	Value
Distribution	Gaussian
N	10^4
Input mean diameter $\langle\sigma\rangle$	1.0
Input standard deviation Δ	0.11
Measured mean diameter $\langle\sigma\rangle$	0.9986221745866380
Measured mean squared diameter $\langle\sigma^2\rangle$	1.0091610833252593
Measured minimum diameter $\sigma_{\min}$	0.5608086811103459
Measured maximum diameter $\sigma_{\max}$	1.4442154686639006

Dim	Model	Dynamics	PolyDisp	N	Density	vol Fr. ϕ	T
2	WCA	isokinetic NVT MD (Brown and Clarke)	11%	10000	0.50-1.10		0.025-5.00

Time scales

MSD



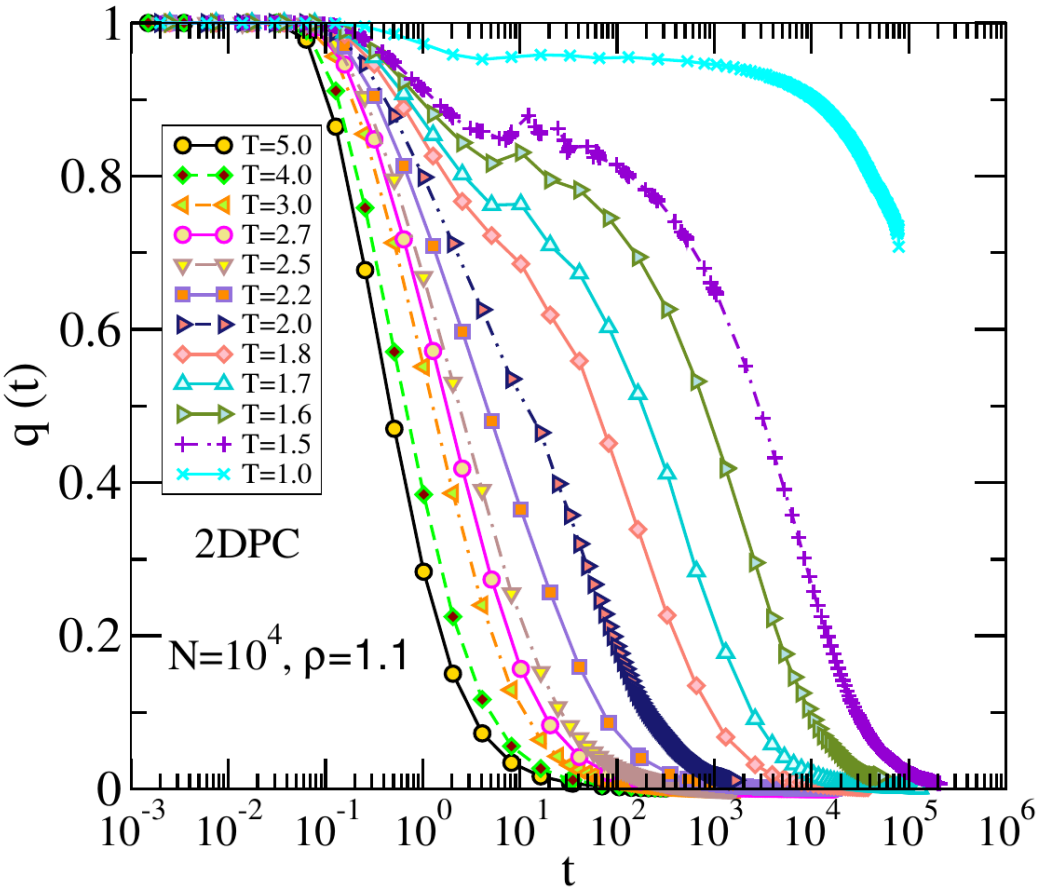


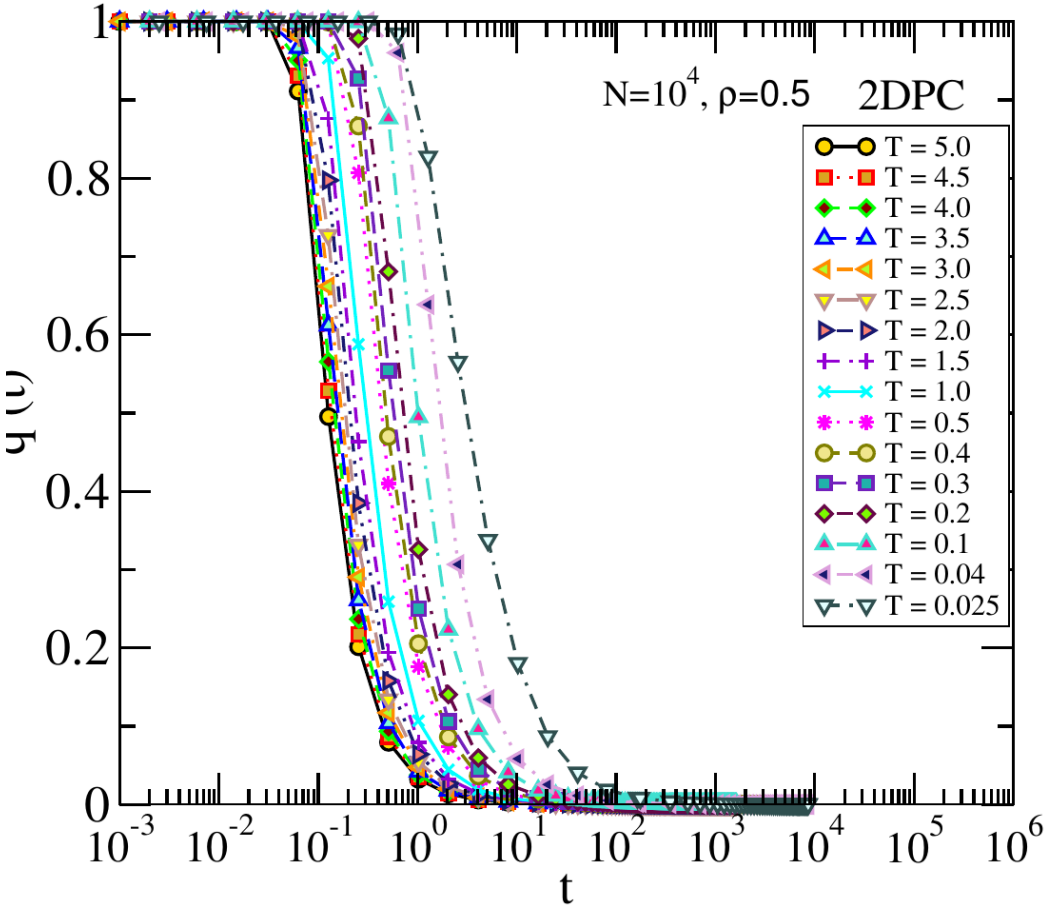
High density

Low density

Time scales

Overlap function



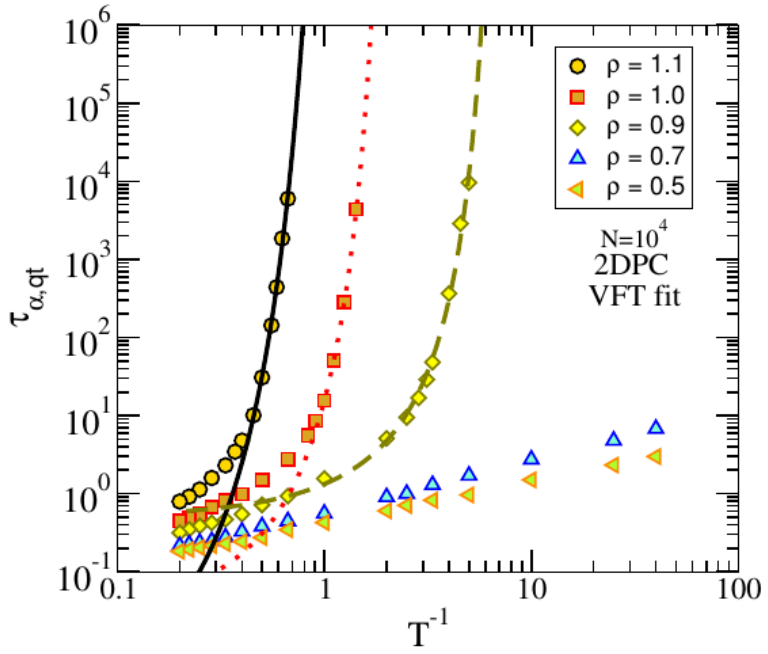


High density

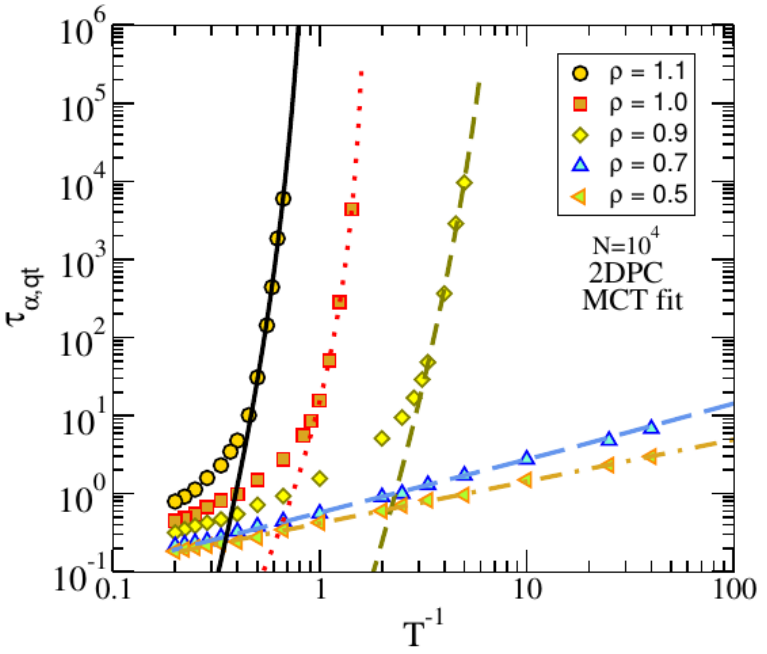
Low density

Temperature scales

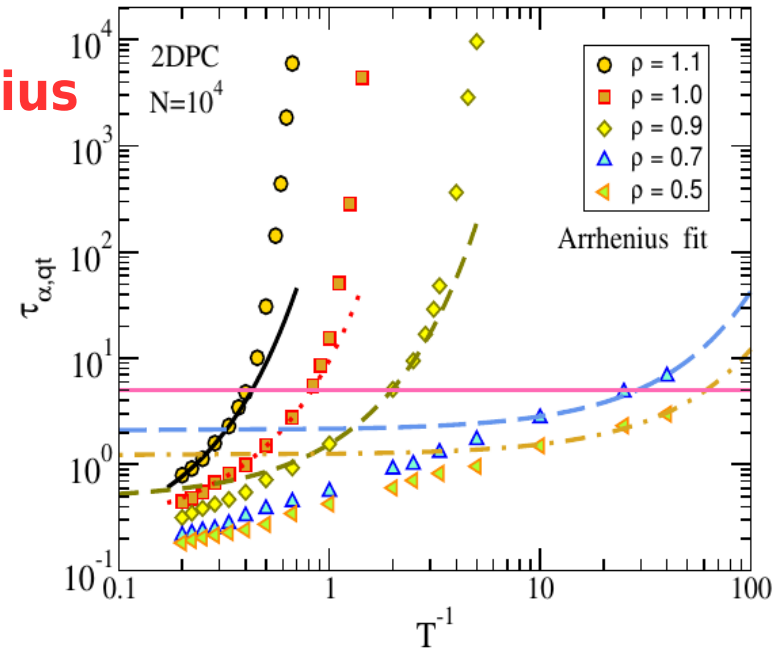
VFT



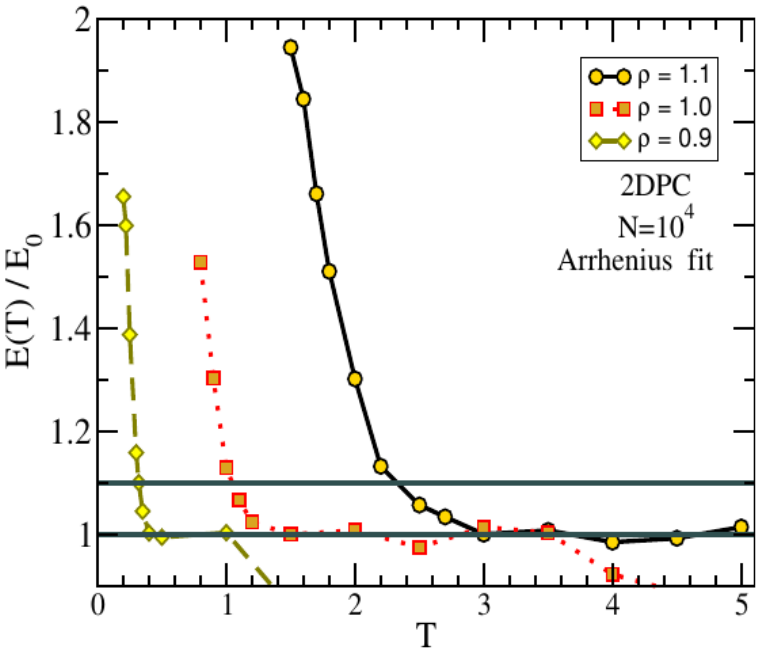
MCT



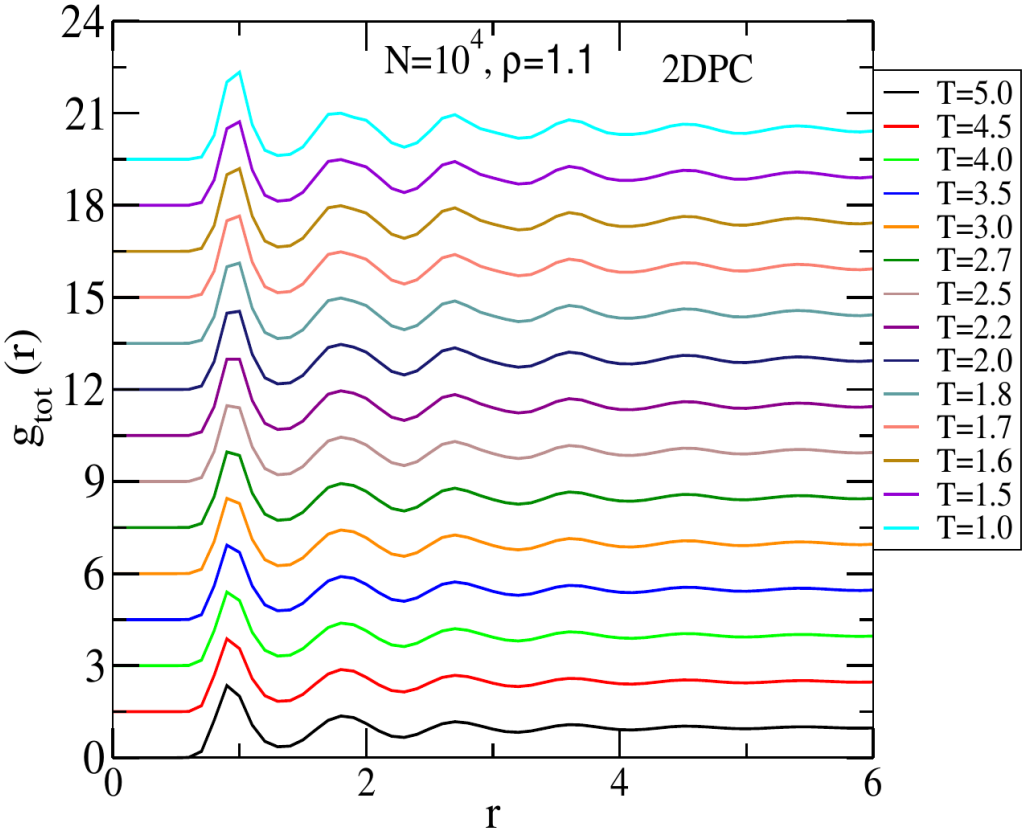
Arrhenius

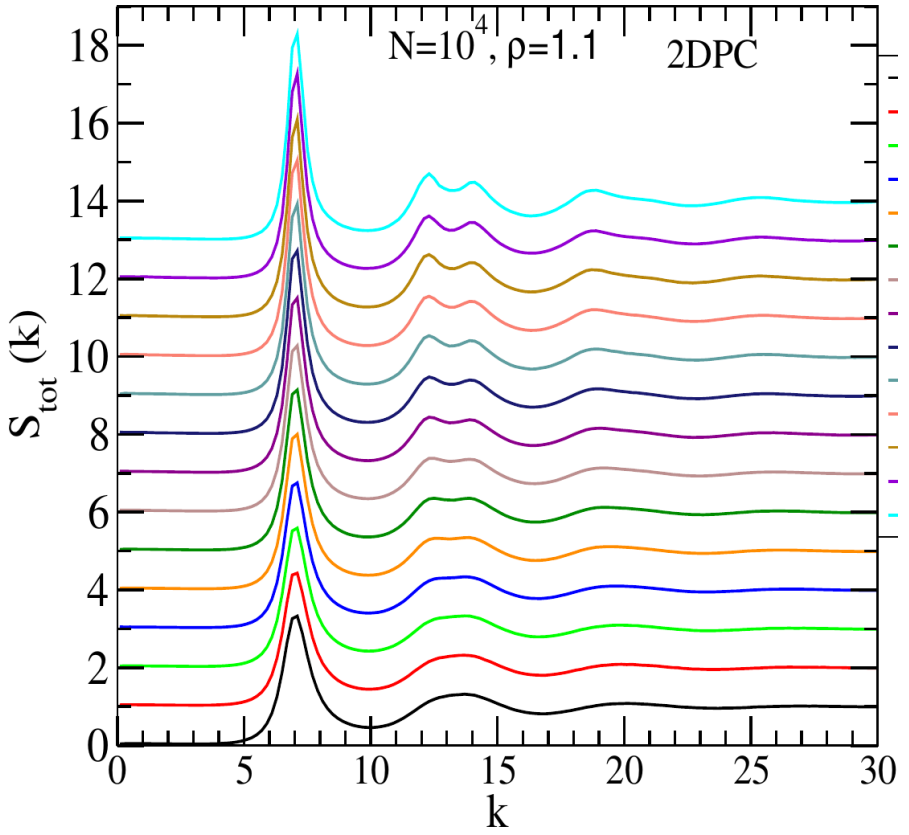


Activation energy

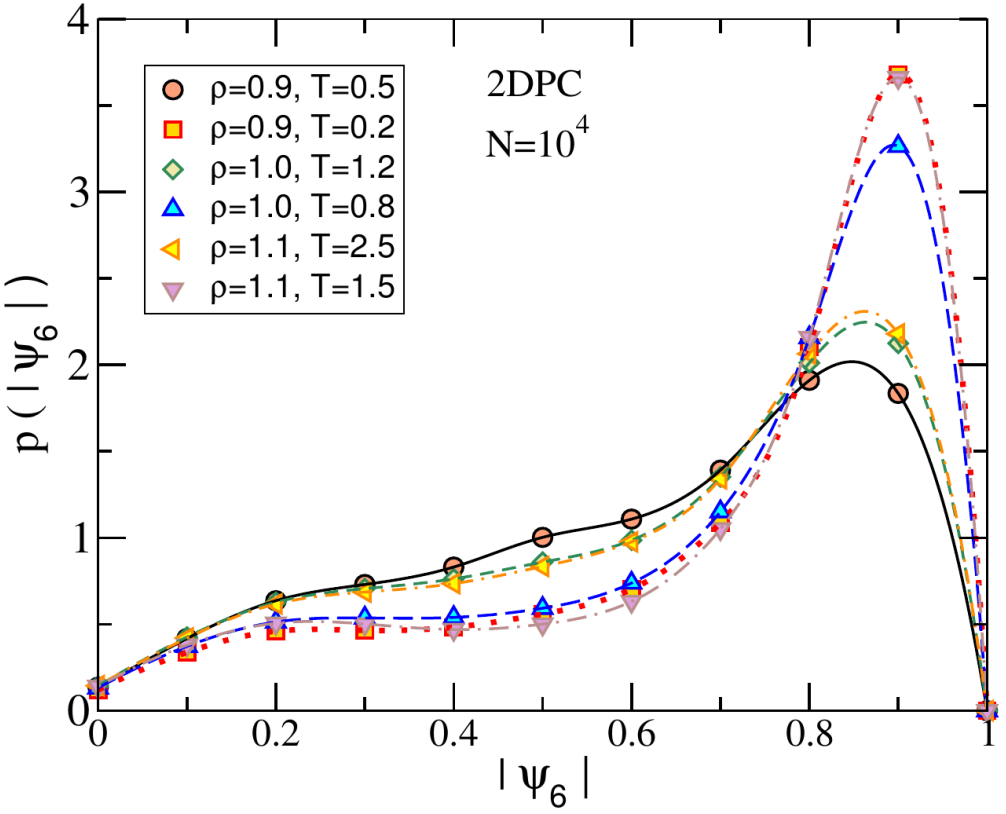


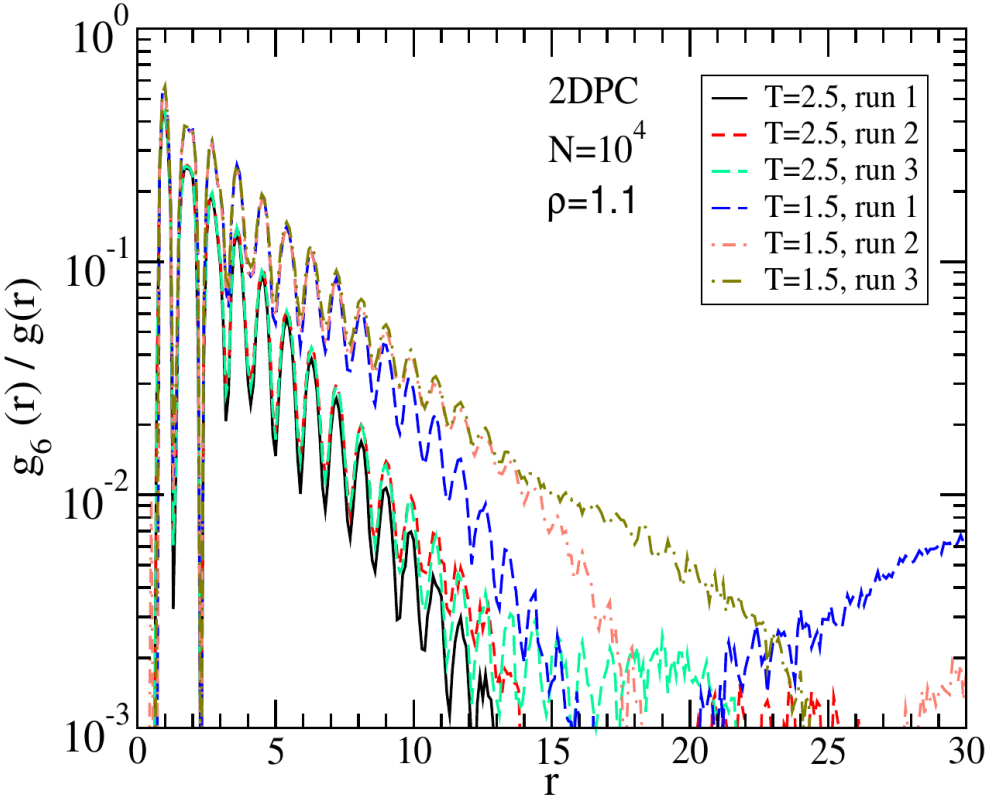
Structure


N=10^4, ρ=1.1
2DPC
T=5.0
T=4.5
T=4.0
T=3.5
T=3.0
T=2.7
T=2.5
T=2.2
T=2.0
T=1.8
T=1.7
T=1.6
T=1.5
T=1.0
g_tot (r)
r


N=10^4, ρ=1.1
2DPC
S_tot (k)
k

Structure

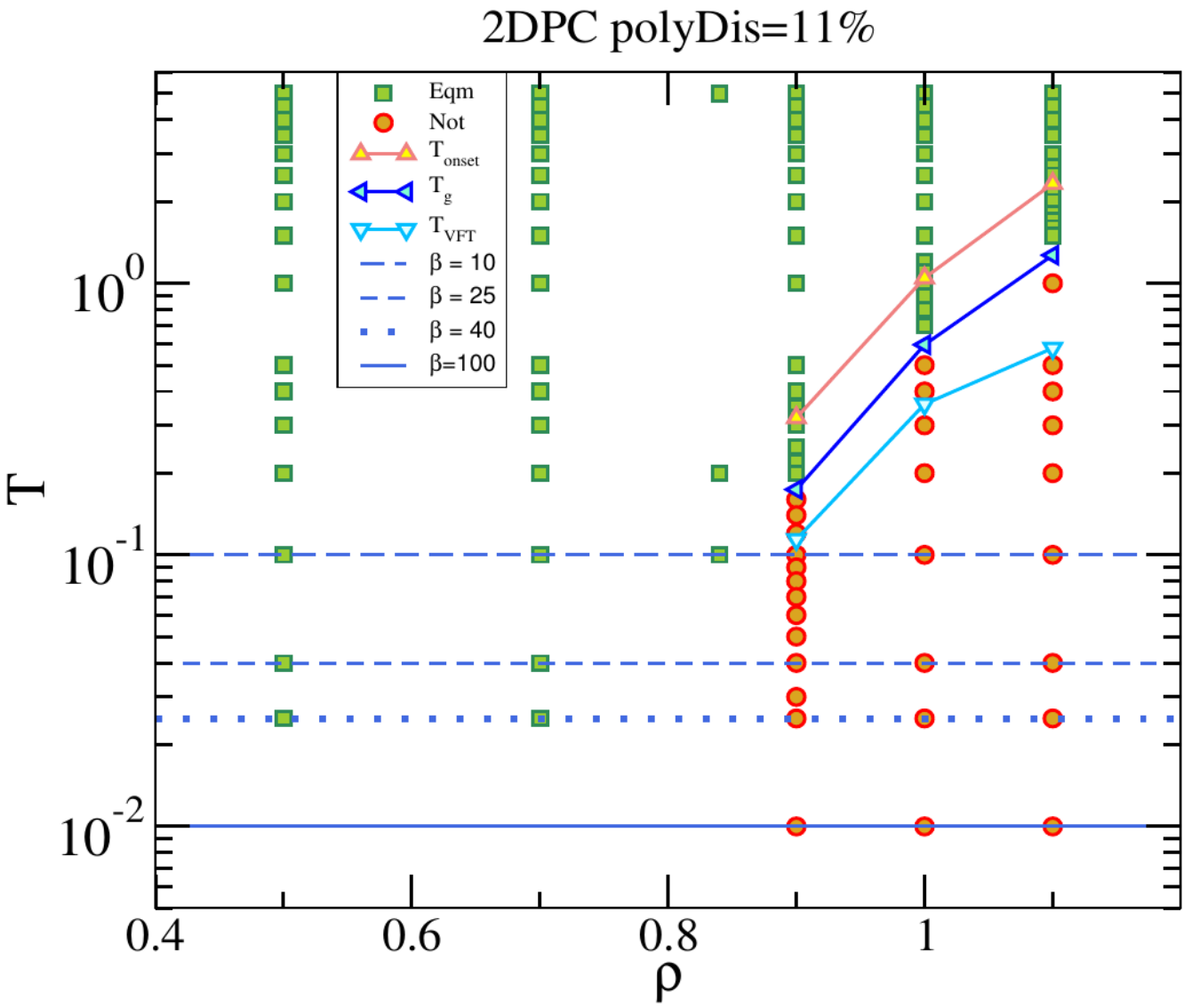




No crystallization even at highest density for this polydispersity

Summary so far

T-ρ phase behaviour



Non-eqm simulation details

Quench protocol

- ***t=0*** *config. from a well-equilibrated run at high* $T\ (=T_h)$
- ***Infinite quench*** *to a target* $T < T_g$
- ***Age*** *system for a duration* t_{age}
- ***Switch on shear at constant strain rate*** $\dot{\gamma}$
- ***Apply shear*** *for another interval* t_{age}

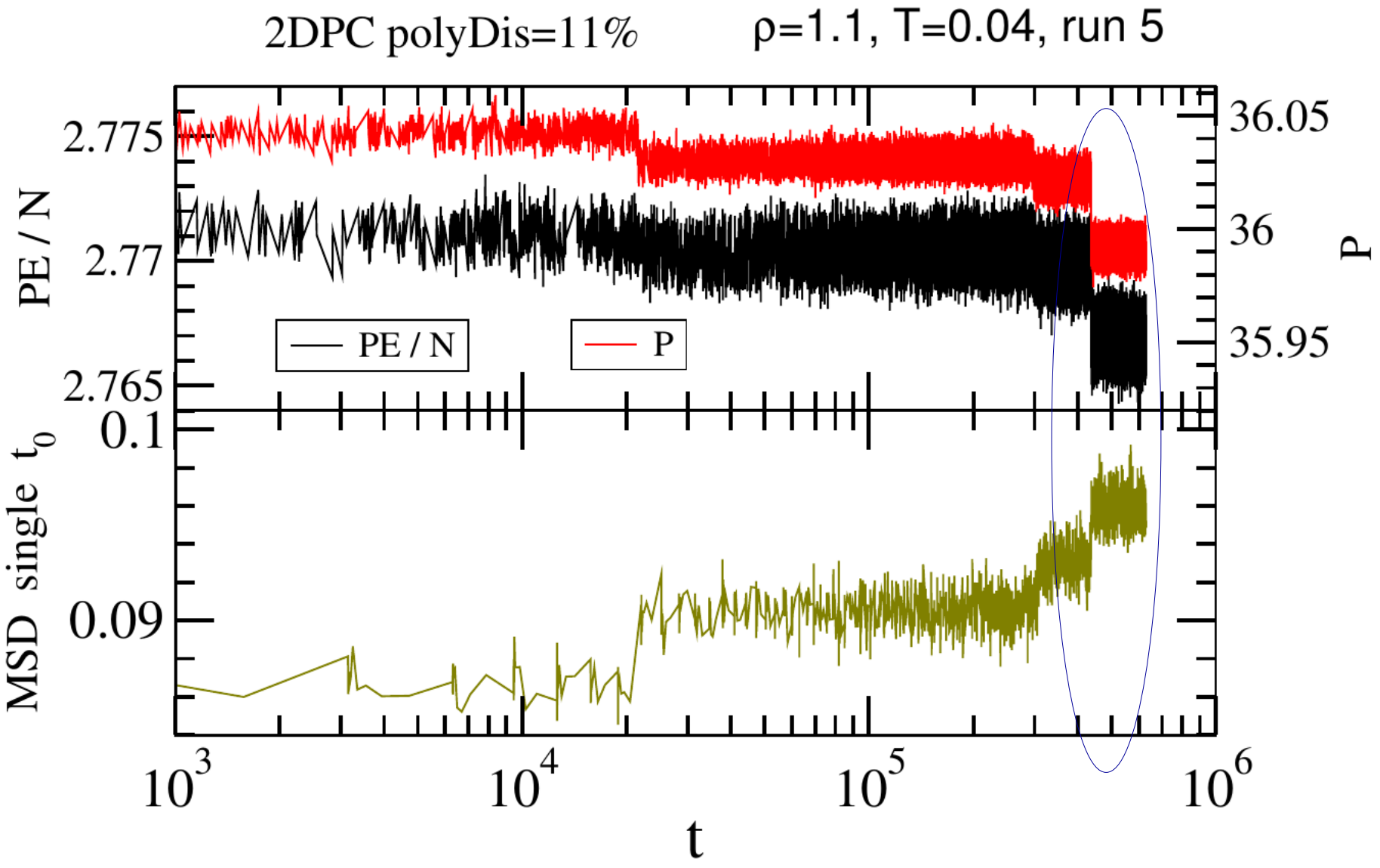
PolyDisp	Density	T_h	t_{age}	$\dot{\gamma}$
11 %	1.10	2.5	6.3×10^5	$10^{-10} - 10^{-3}$
	1.00	1.2	6.3×10^5	$10^{-10} - 10^{-3}$
	0.90	0.5	6.3×10^5	$10^{-10} - 10^{-3}$

Avalanche: indicators

Particle averaged indicators

- ***Sharp drop in per particle potential energy***
- ***Sharp drop in pressure***
- ***Sharp rise in squared displacement (particle averaged but not time origin averaged)***

Avalanche: indicators

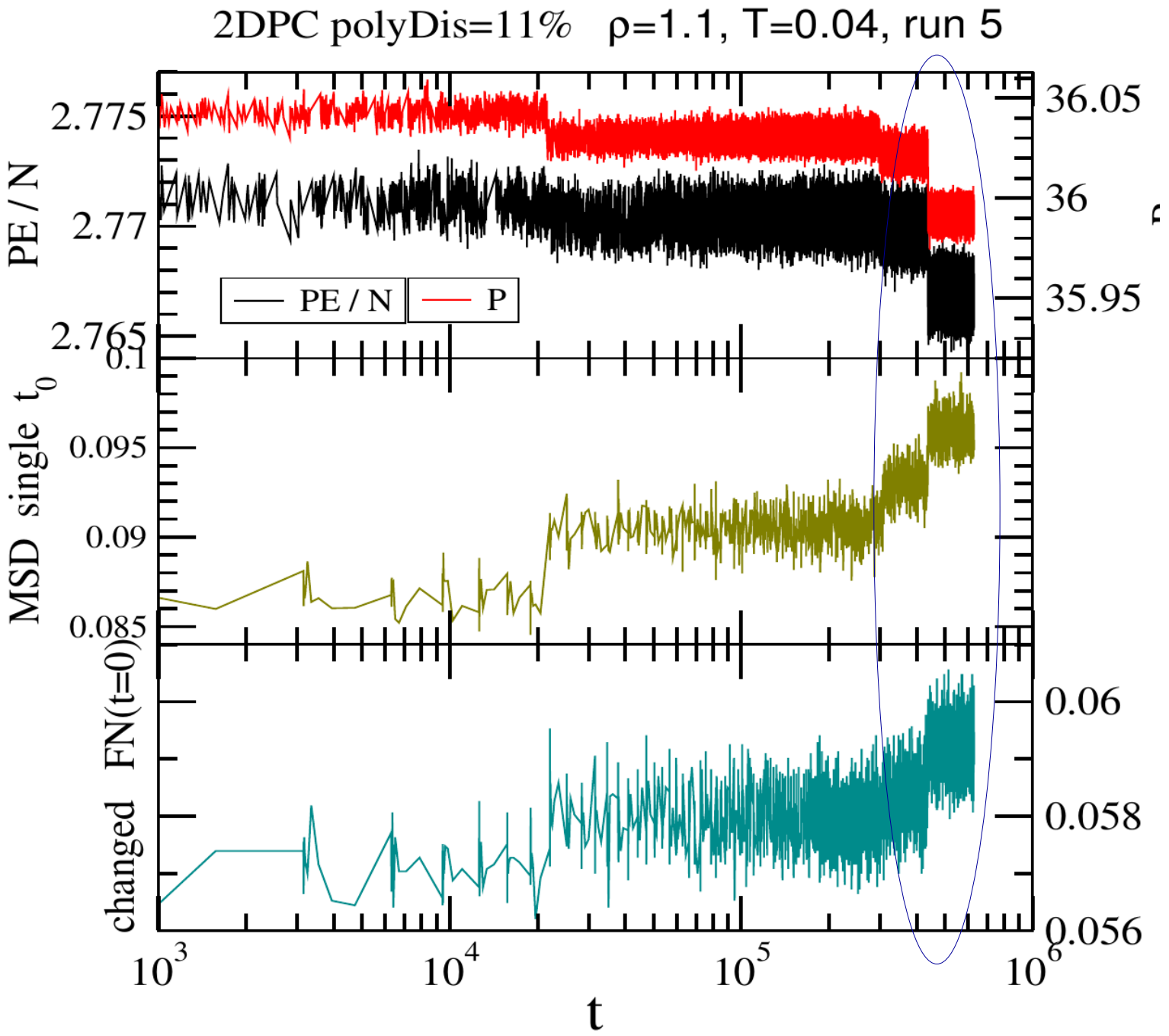


Avalanche: indicators

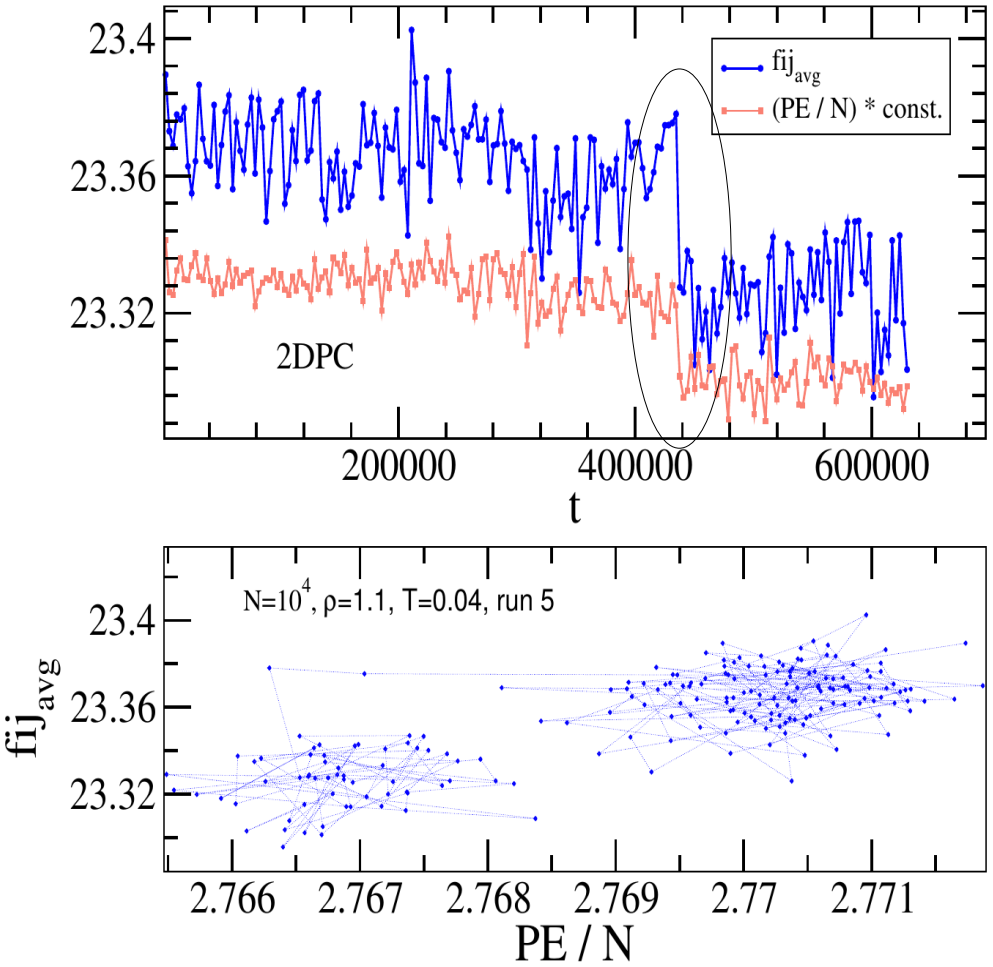
Re-wiring of force network

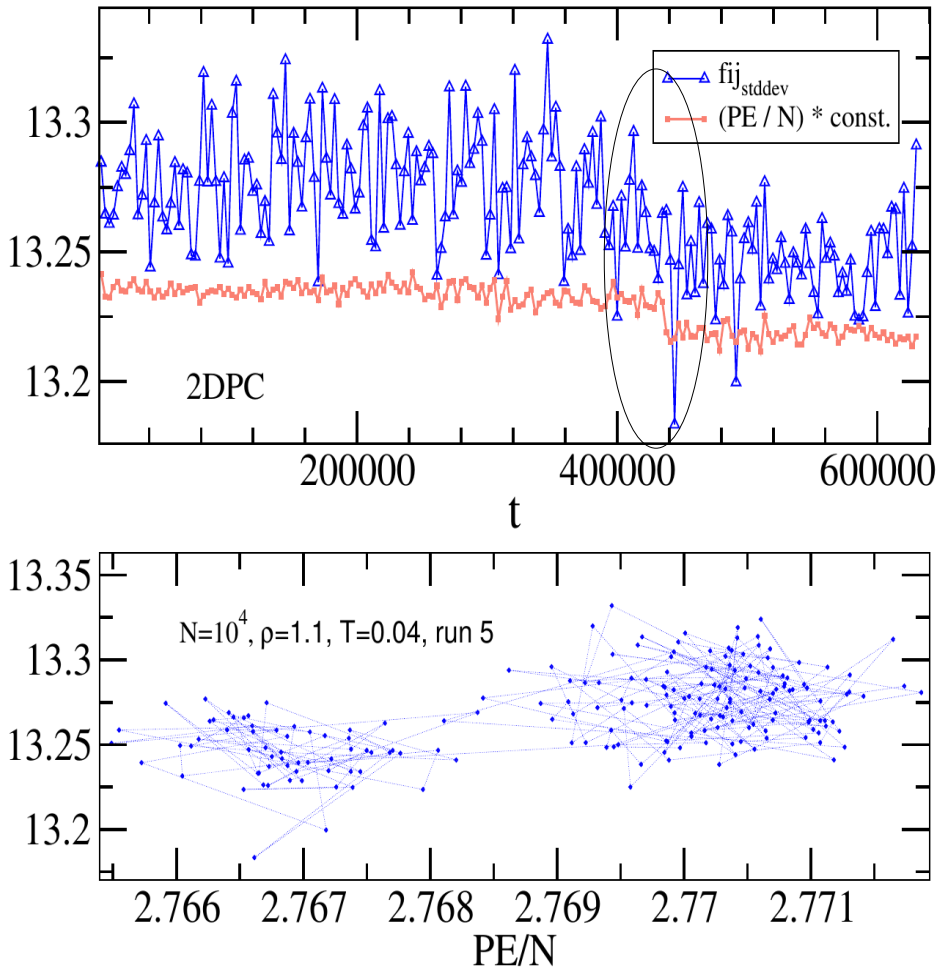
- ***Sharp rise in fraction of initial force neighbours lost***
- ***Sharp drop in average value of contact force distribution***
- ***Sharp drop in standard deviation of contact force distribution***

Avalanche: indicators



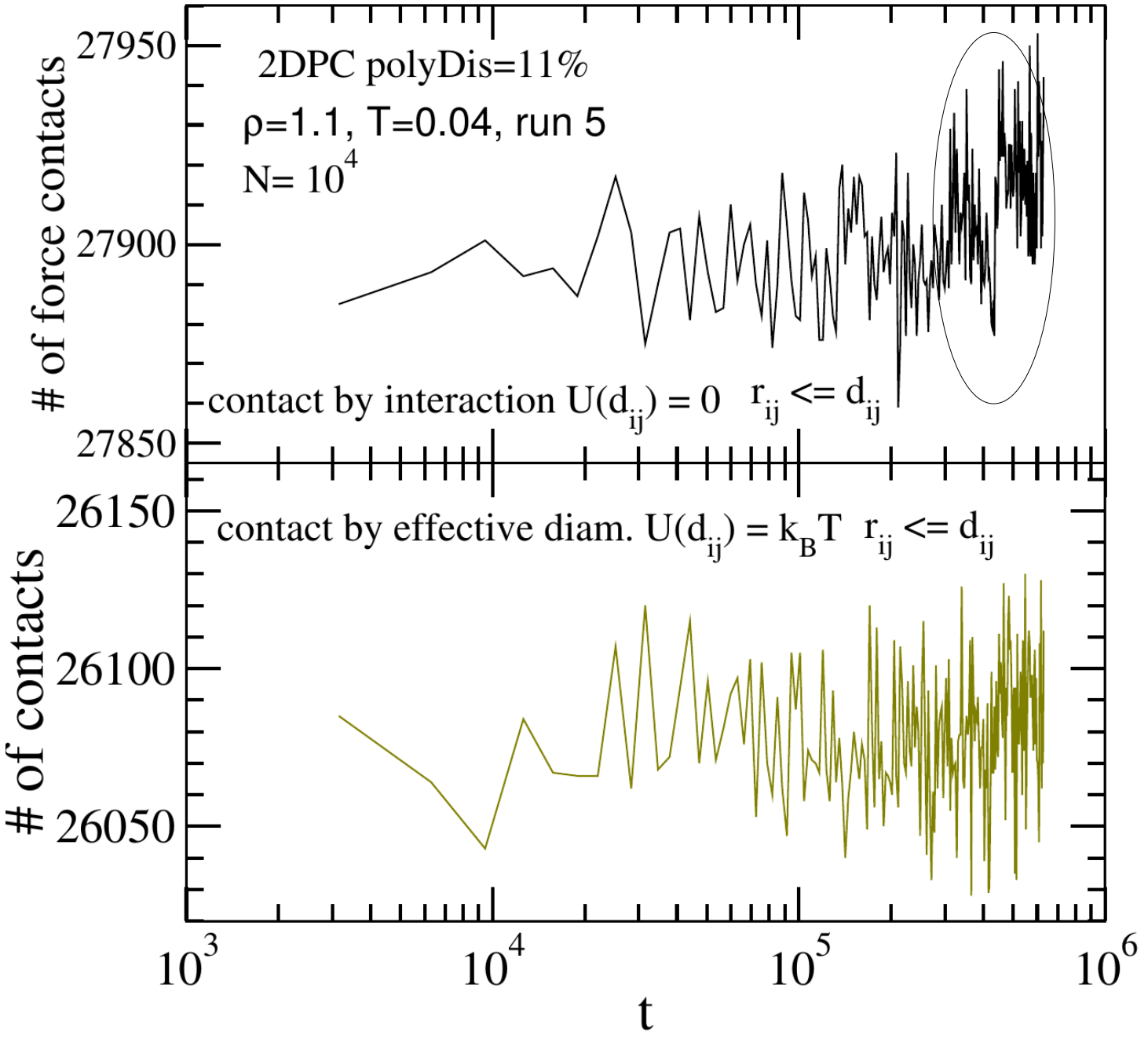
Avalanche: indicators



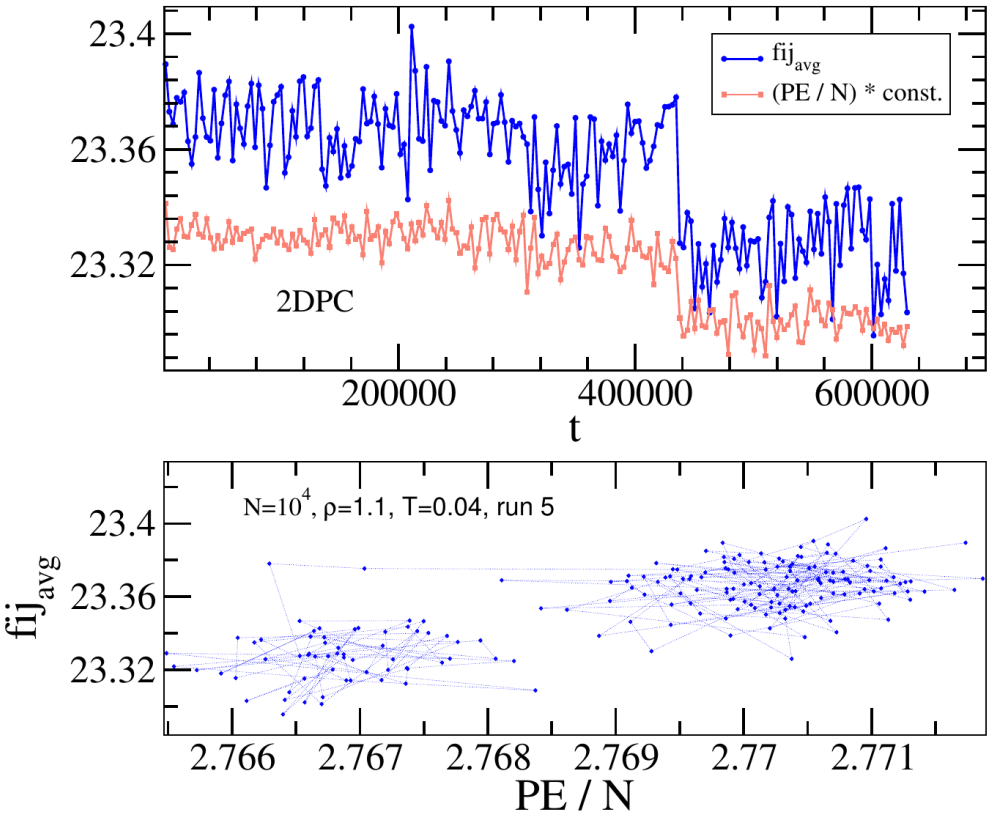


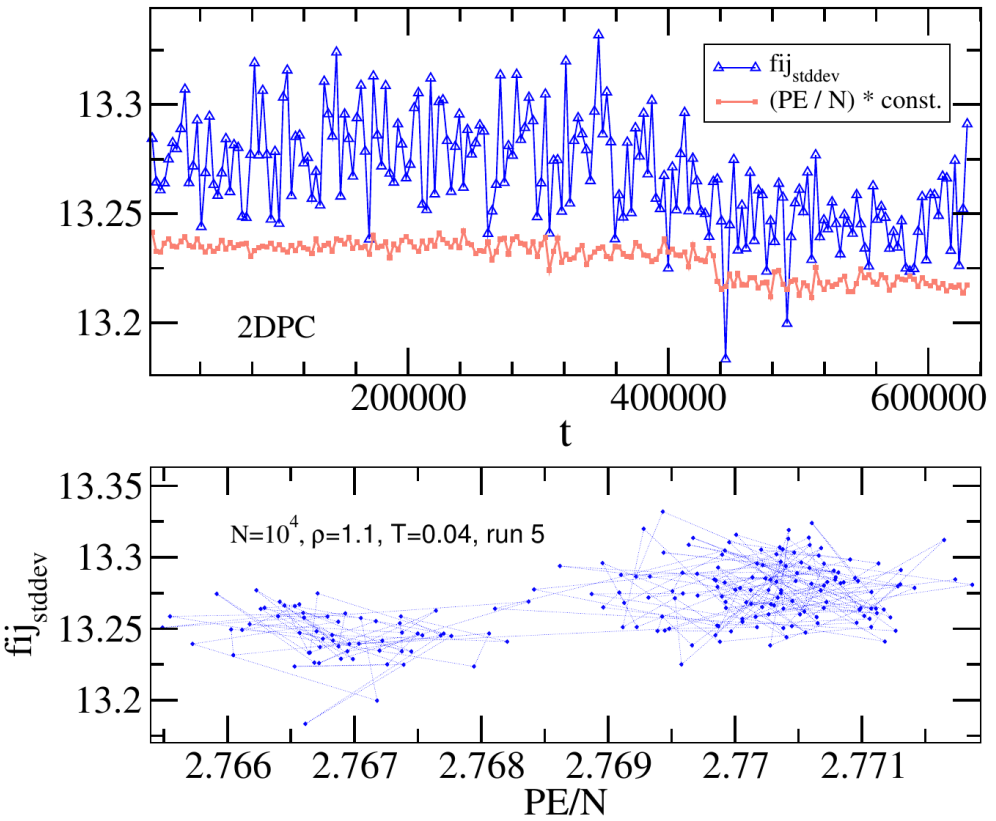
Average **Std. dev.**

Avalanche: indicators



Avalanche: indicators



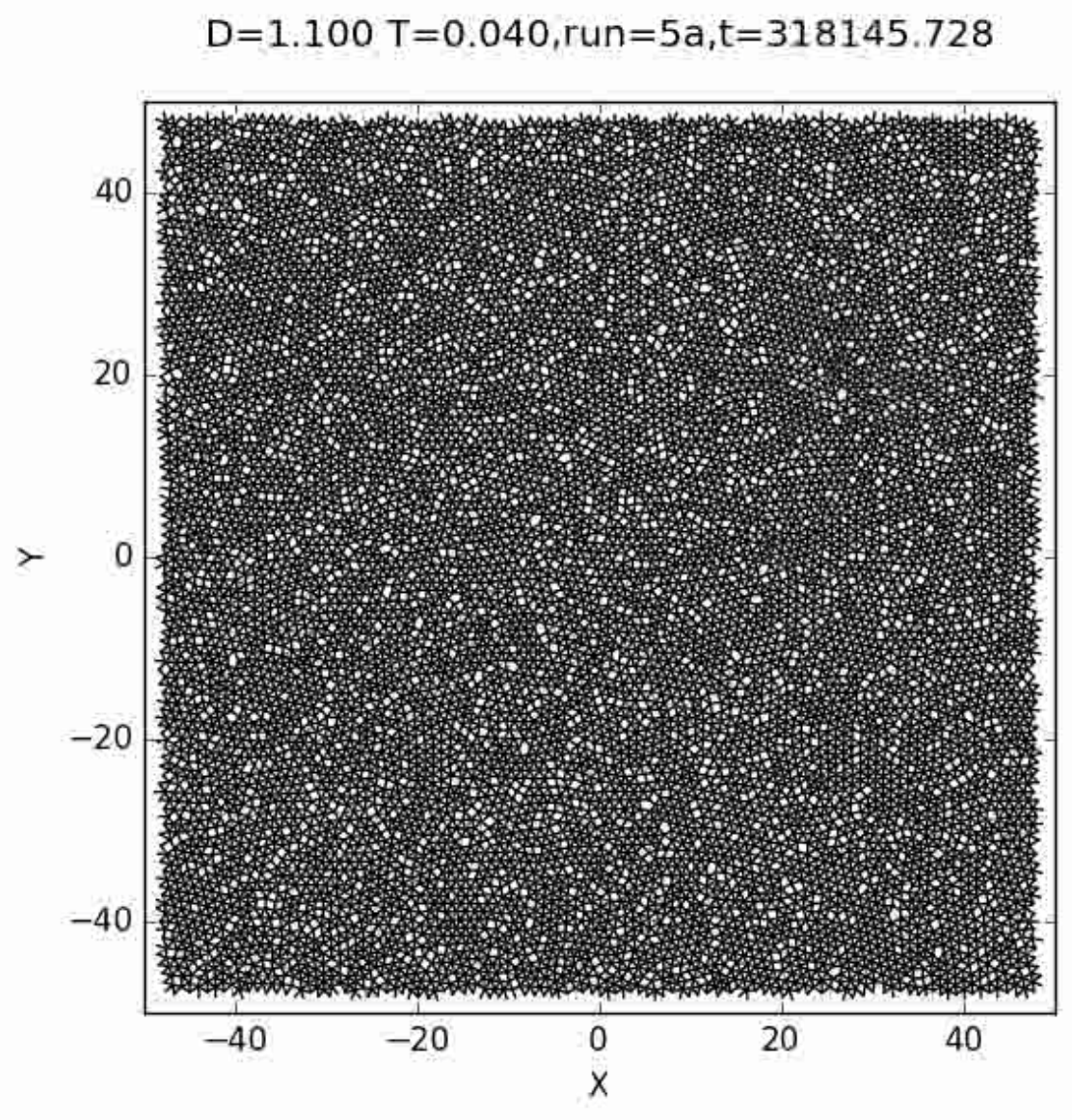


Average

Std. dev.

Avalanche: indicators

Visualization



Summary, future plans

We have taken a model, almost hard-sphere like glass in 2D.

Calculated the T-rho phase diagram at fixed polydispersity to identify the “glassy” regime.

Avalanche events are analyzed in real space.

Next step is to switch on shear and determine selection rules for avalanche initiator particles under shear.

Thank you ! Questions ???