Time dependent elastic response to a local shear transformation in amorphous solids

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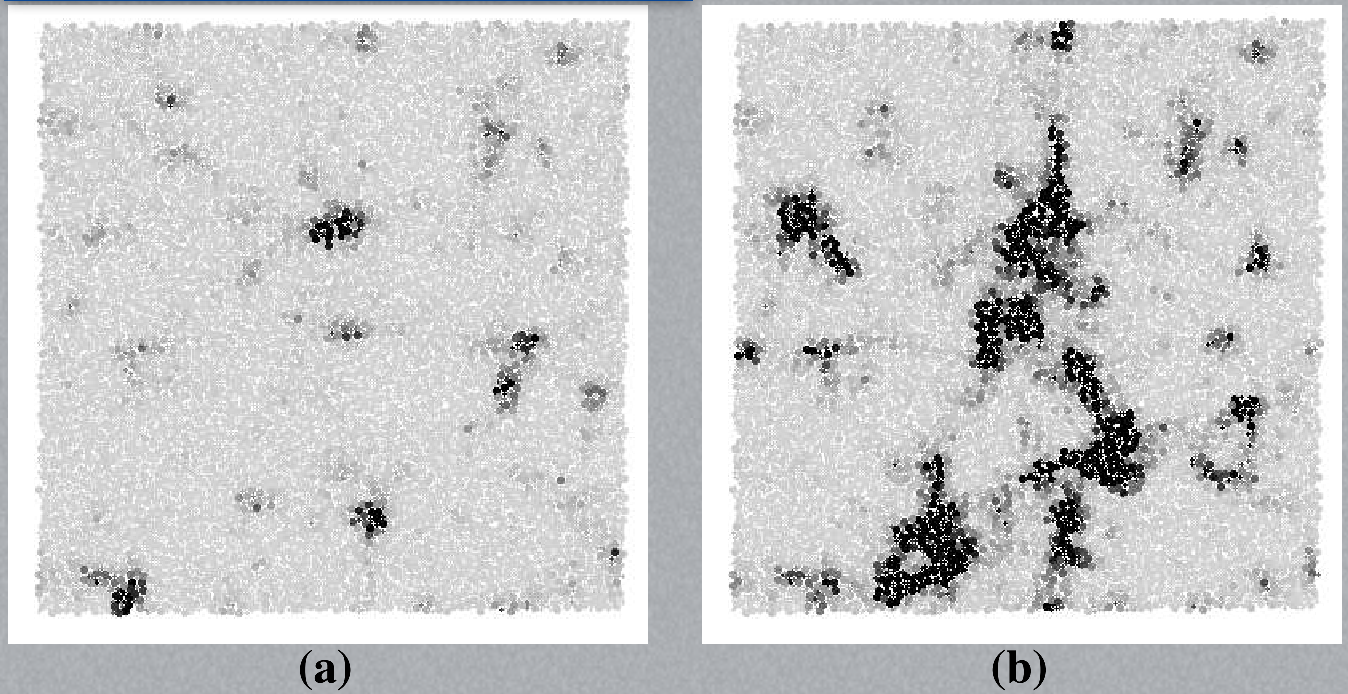
Shear Transformations

At low temperature, the onset of plastic deformation in glasses is due to the accumulation of **elementary plastic events**, consisting of localized in space and time atomic rearrangements involving only a few tens of atoms, the so-called Shear Transformations (STs).

Atomistic simulations of deformation in amorphous solids
Falk and Langer (1998)



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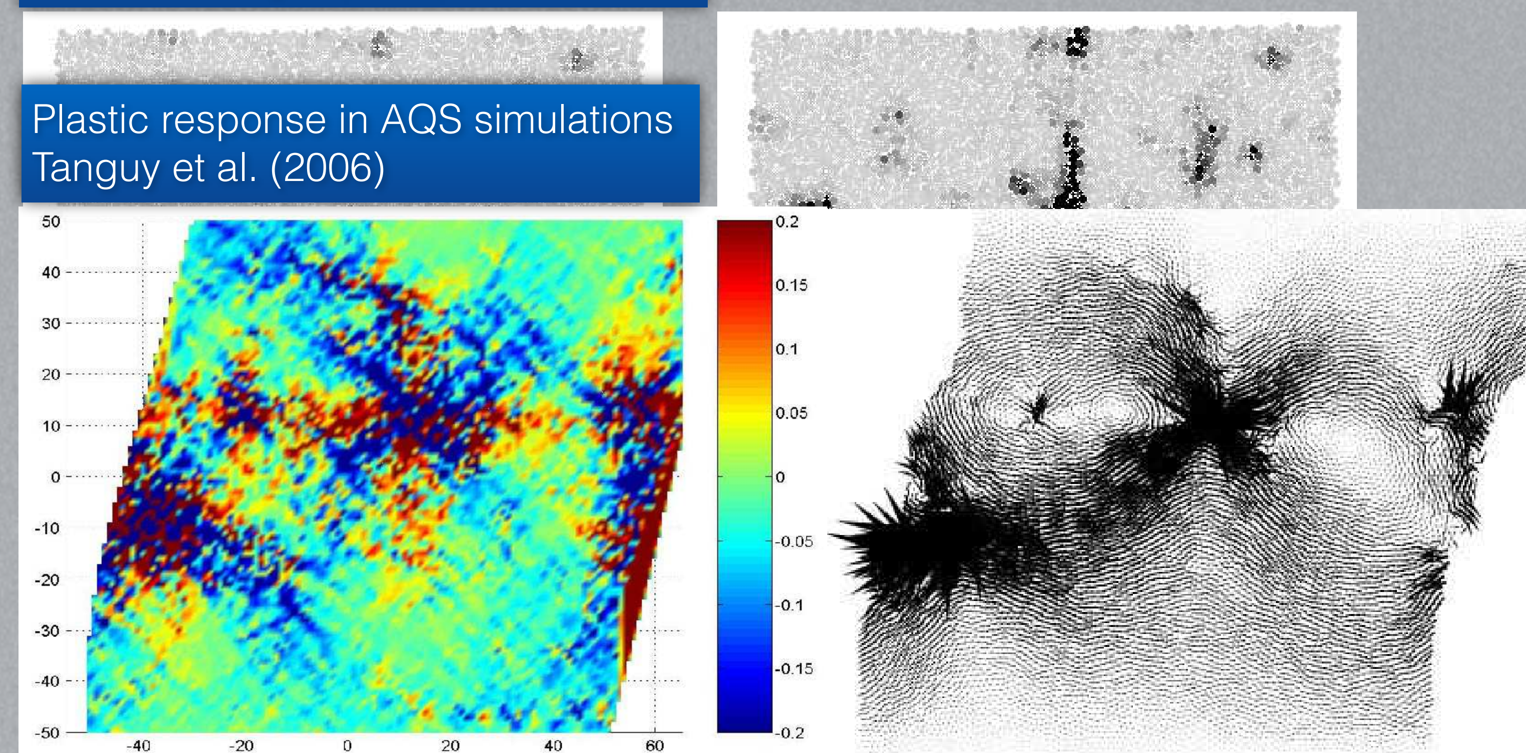
Plastic response in AQS simulations
Tanguy et al. (2006)



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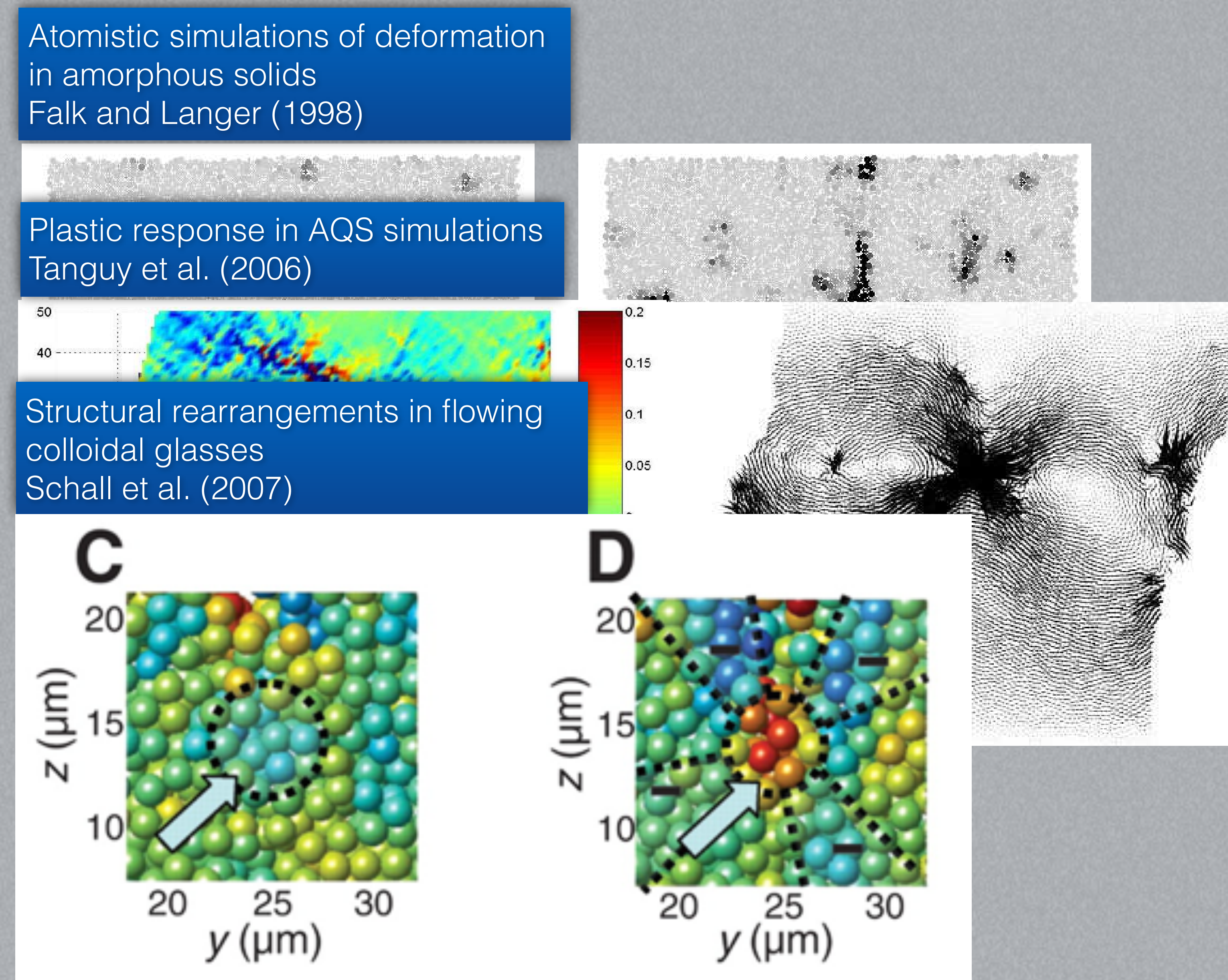

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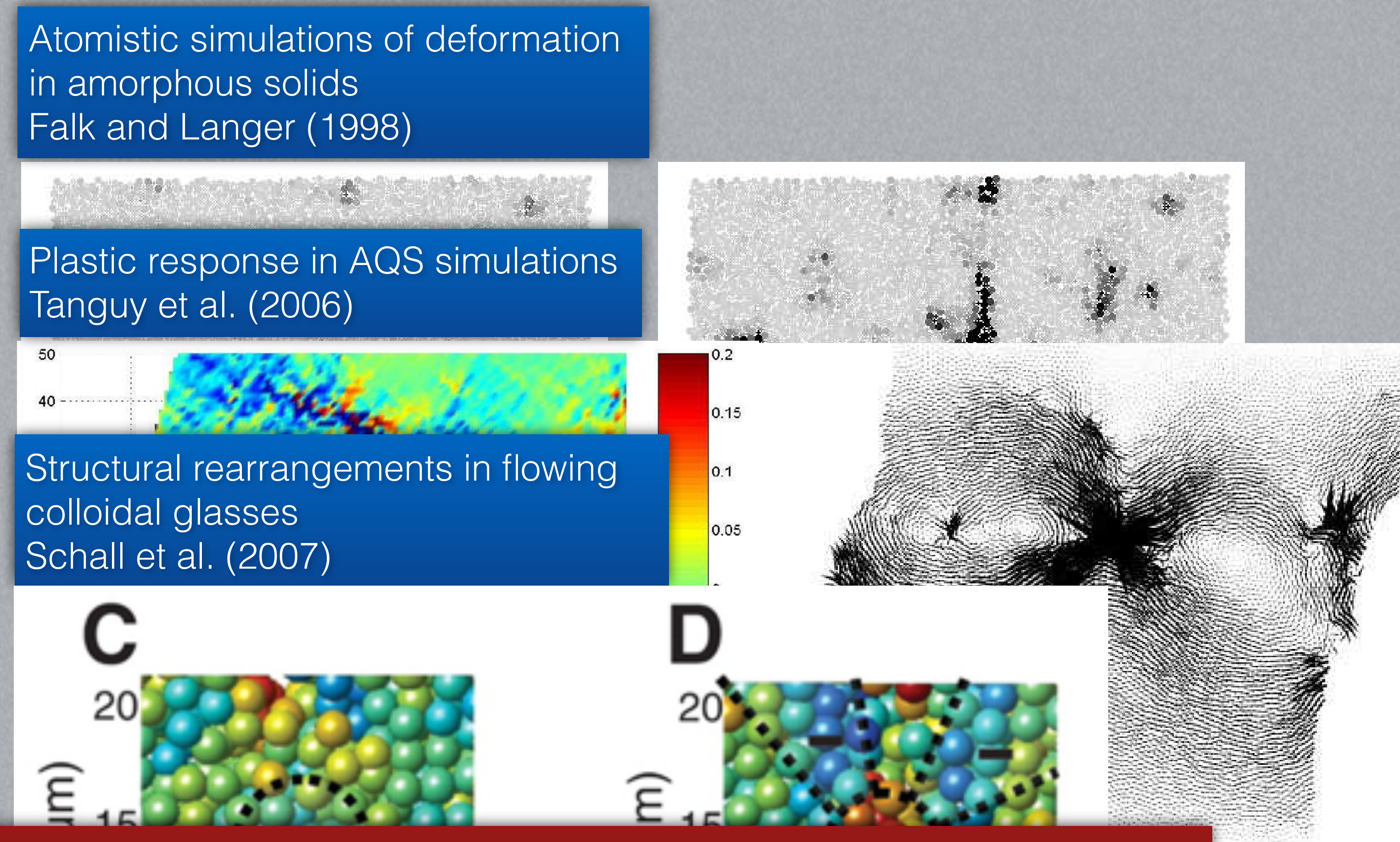


Open questions:

- How does the elastic response to a ST build in time?
- How does inertia affect the response?
- How is the position of a plastic event influenced by that of its predecessors?

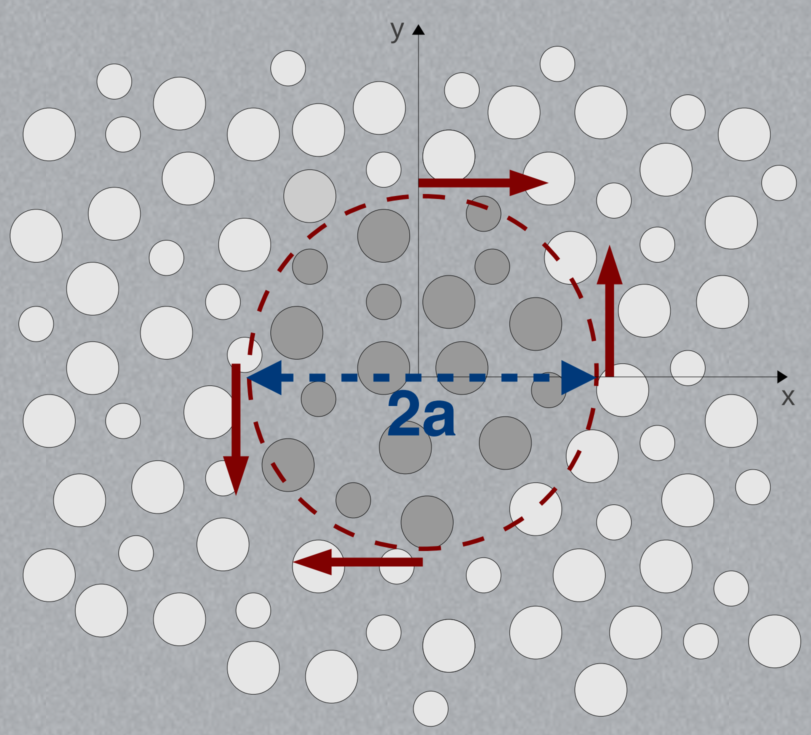
Outline

- Methods
- Equilibrium response to a ST
- Propagation of elastic signal and time dependent solution
- Plastic effects
- Conclusions

Replicating a ST

- 2D binary mixture of Lennard-Jones particles
- T=0 configuration obtained quenching from high T.
- We apply an instantaneous shear transformation to a circular region and observe the response of the system. We set:

  $\epsilon = 2.5 \times 10^{-2} \qquad a = 2.5\,\sigma$



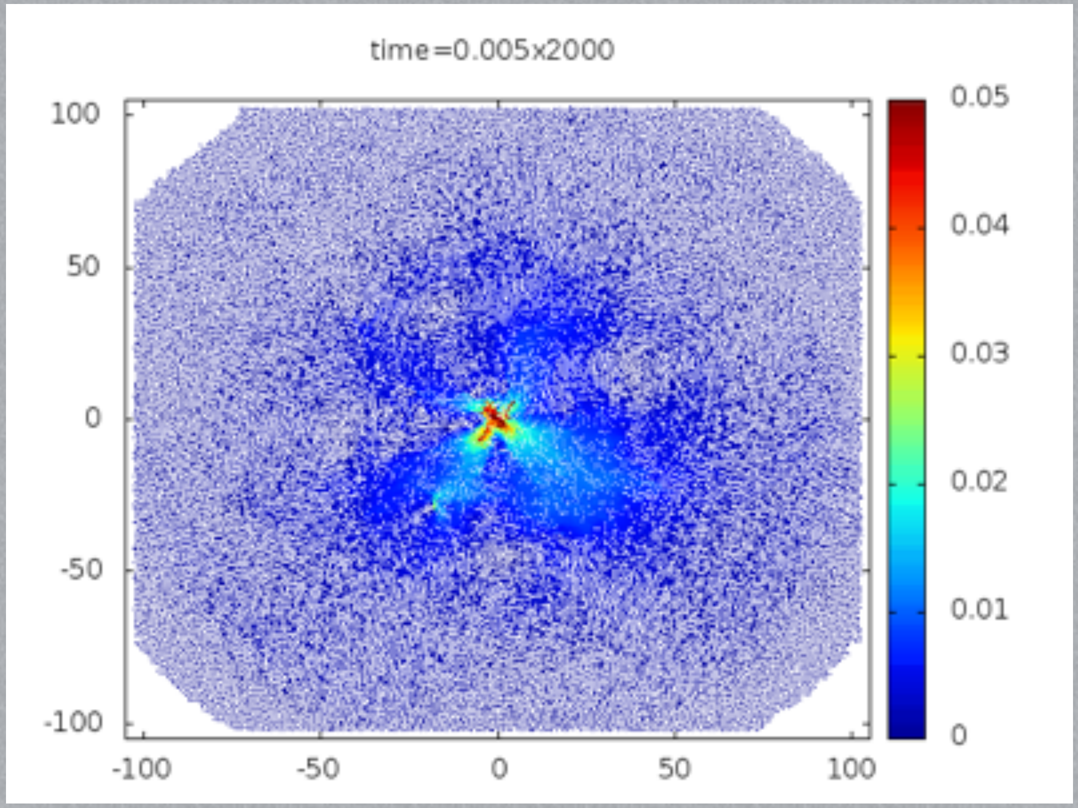
$$\begin{cases} x_i \to x_i' = x + \epsilon y \\ y_i \to y_i' = y + \epsilon x \end{cases}$$

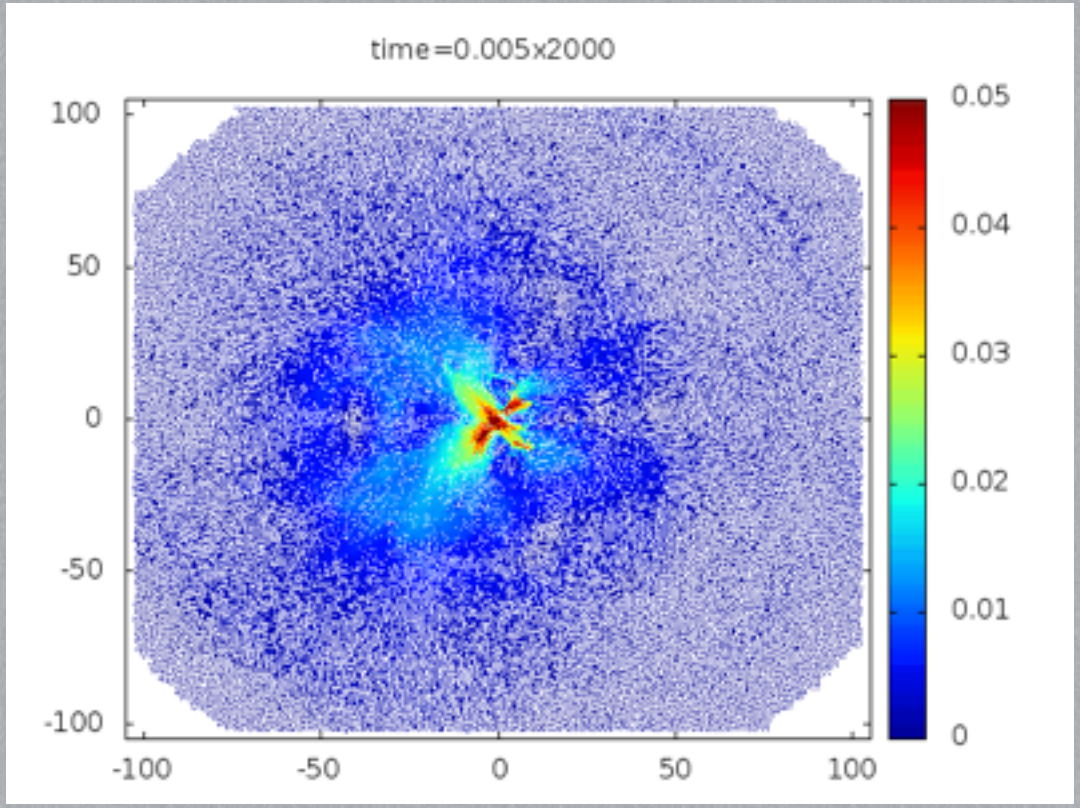
- Langevin thermostat:

$$\begin{aligned} \frac{d\mathbf{r}_i}{dt} &= \frac{\mathbf{p}_i}{m} \\ \frac{d\mathbf{p}_i}{dt} &= -\sum_{j\neq i} \frac{\partial V(\mathbf{r}_{ij})}{\partial \mathbf{r}_{ij}} - \frac{\mathbf{p}_i}{\tau} \end{aligned}$$

As τ decreases, the dynamics changes from **underdamped** to over**damped**

Working out the effects of disorder





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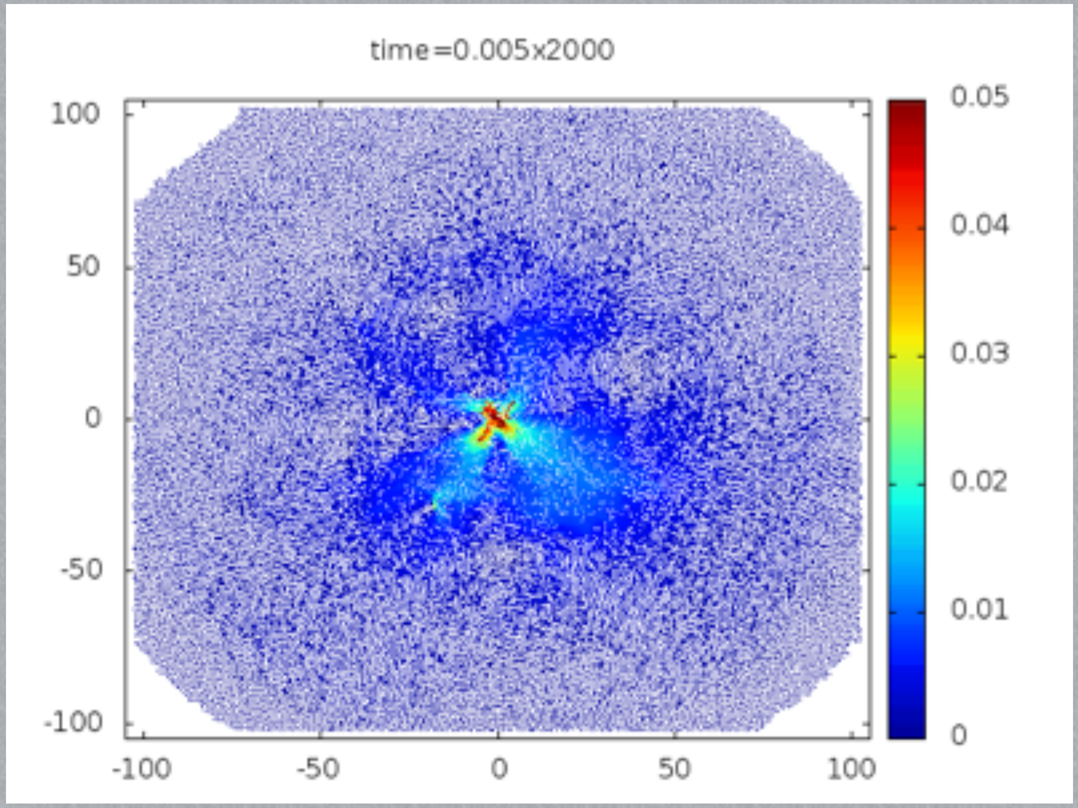

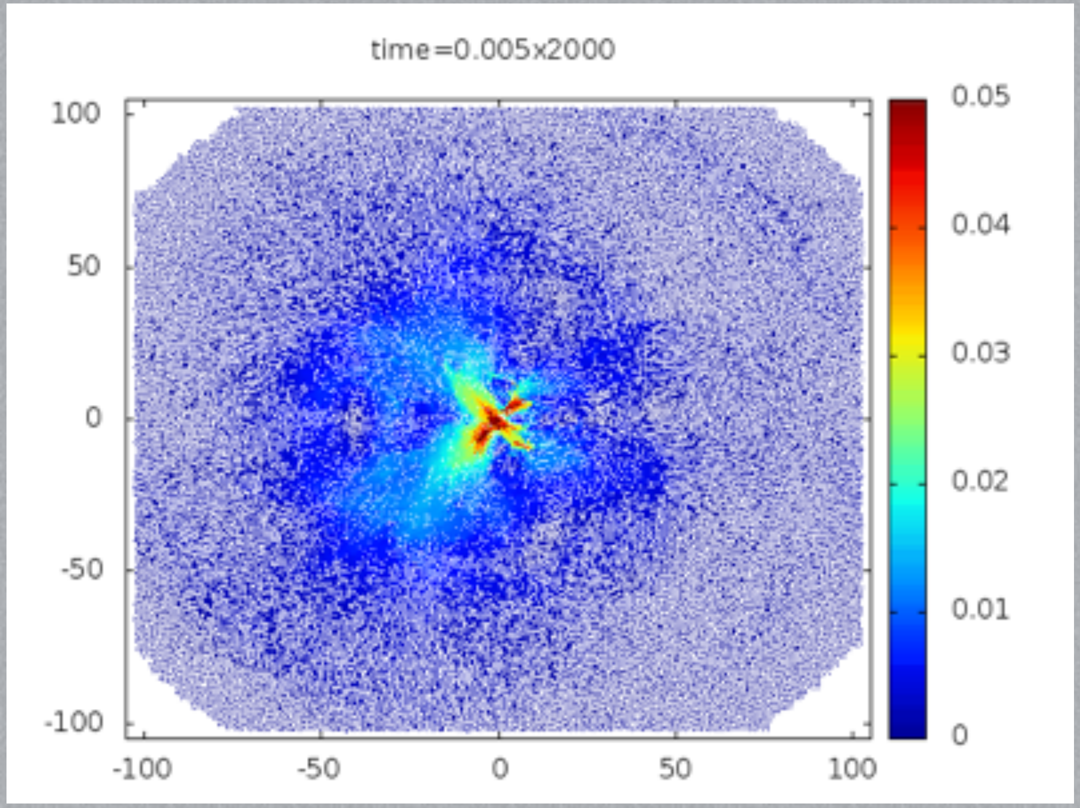

- Following the ST, the elastic signal propagates in the system; at long times a new equilibrium state is achieved.

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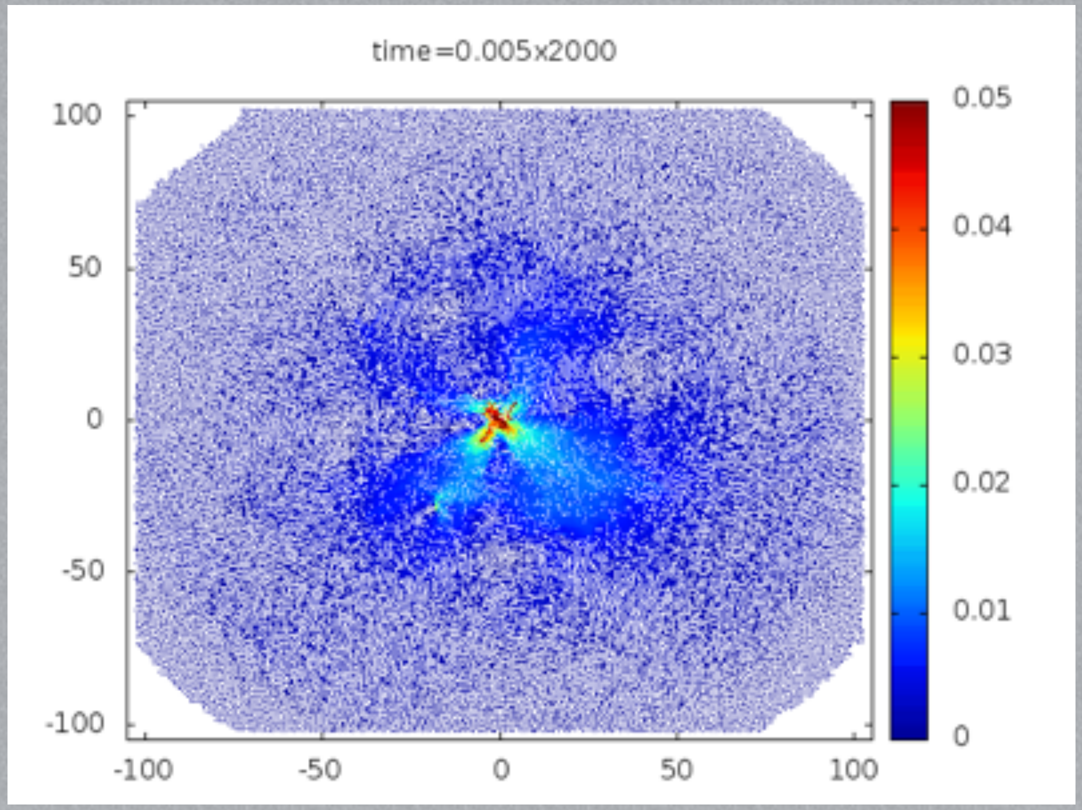

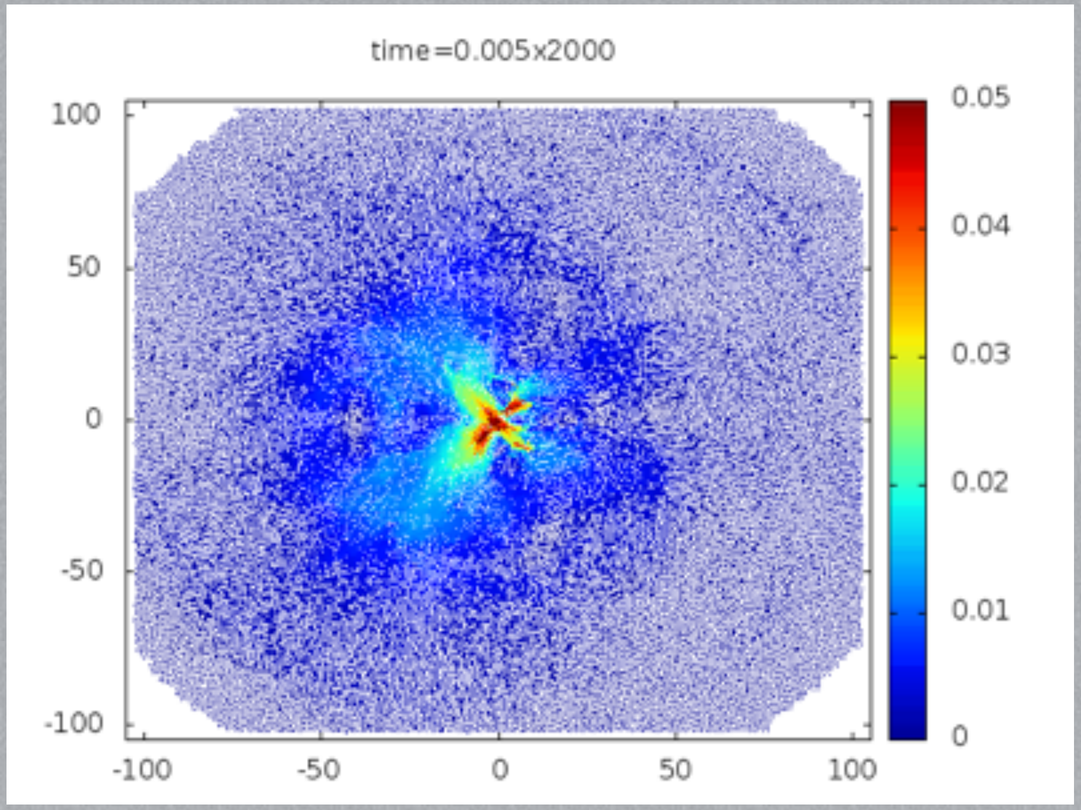

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- Structural disorder strongly affects the transient and equilibrium patterns.

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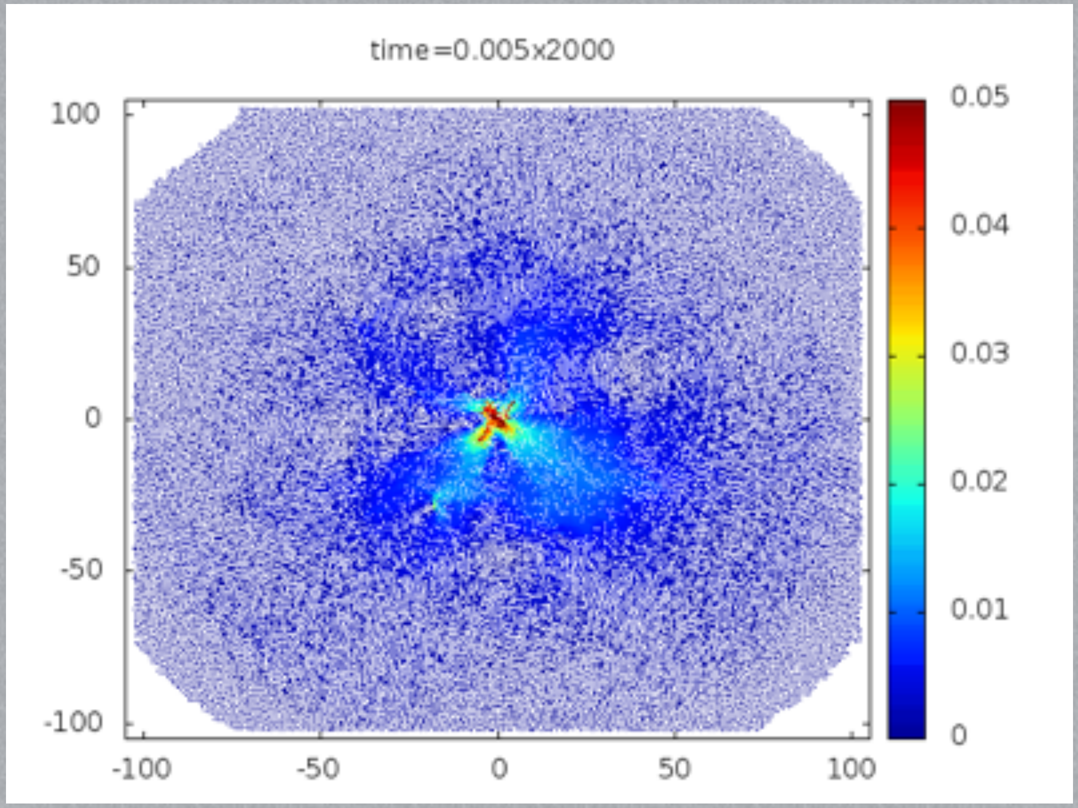

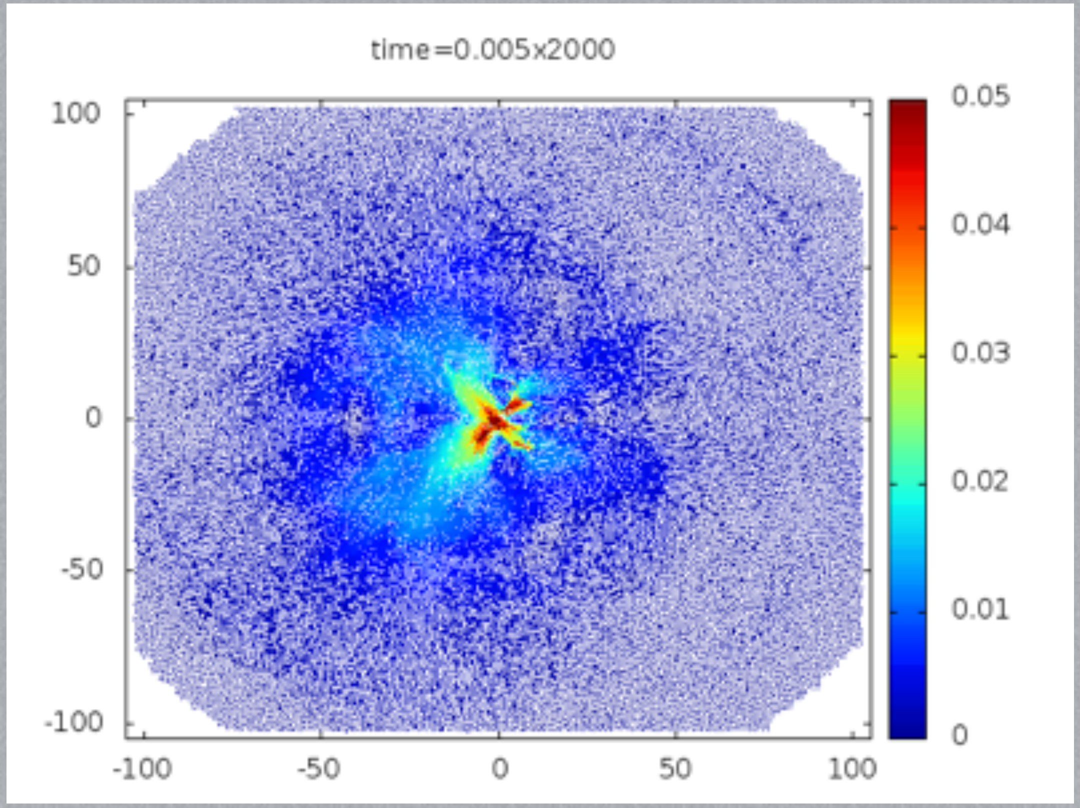

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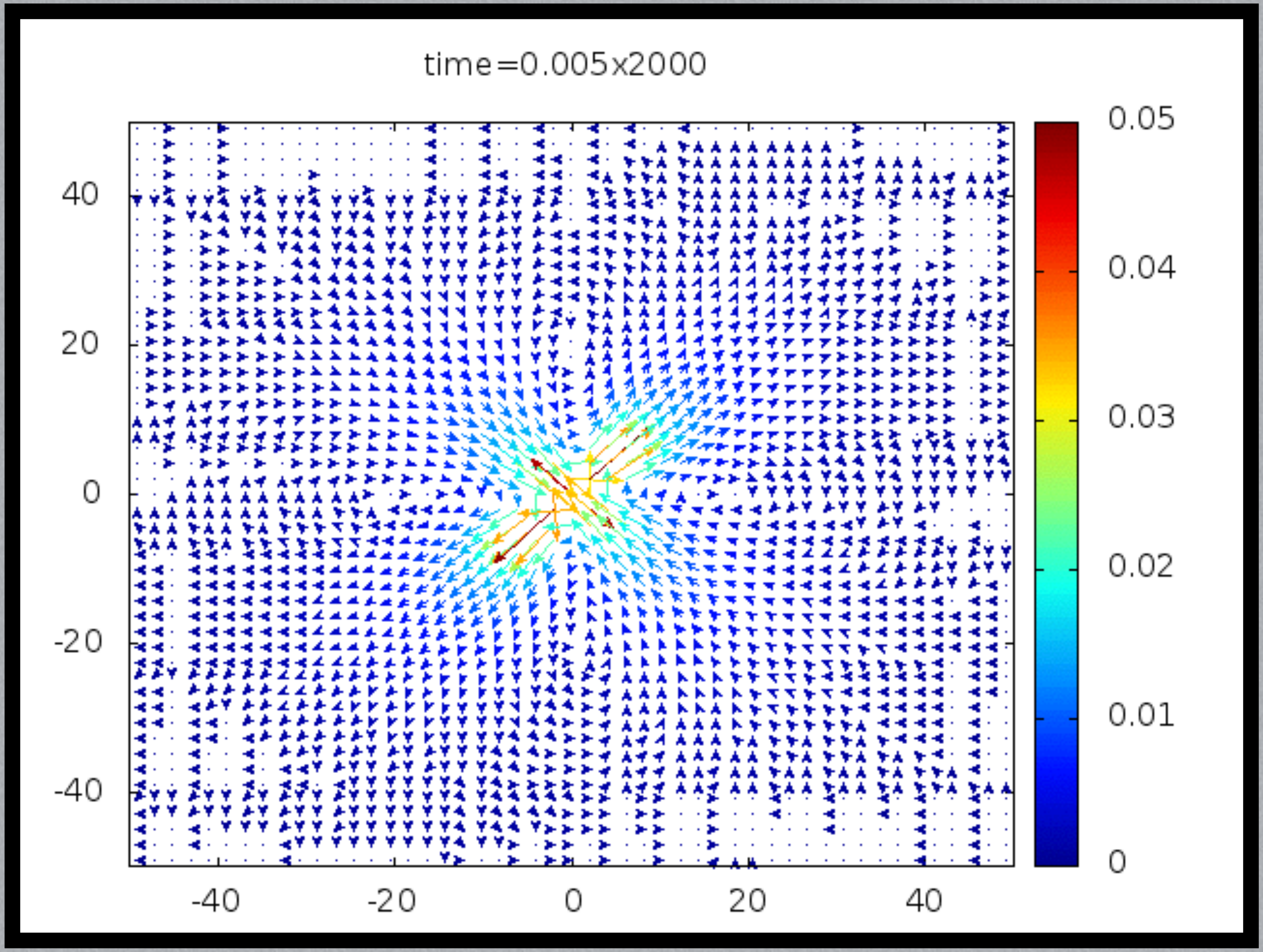

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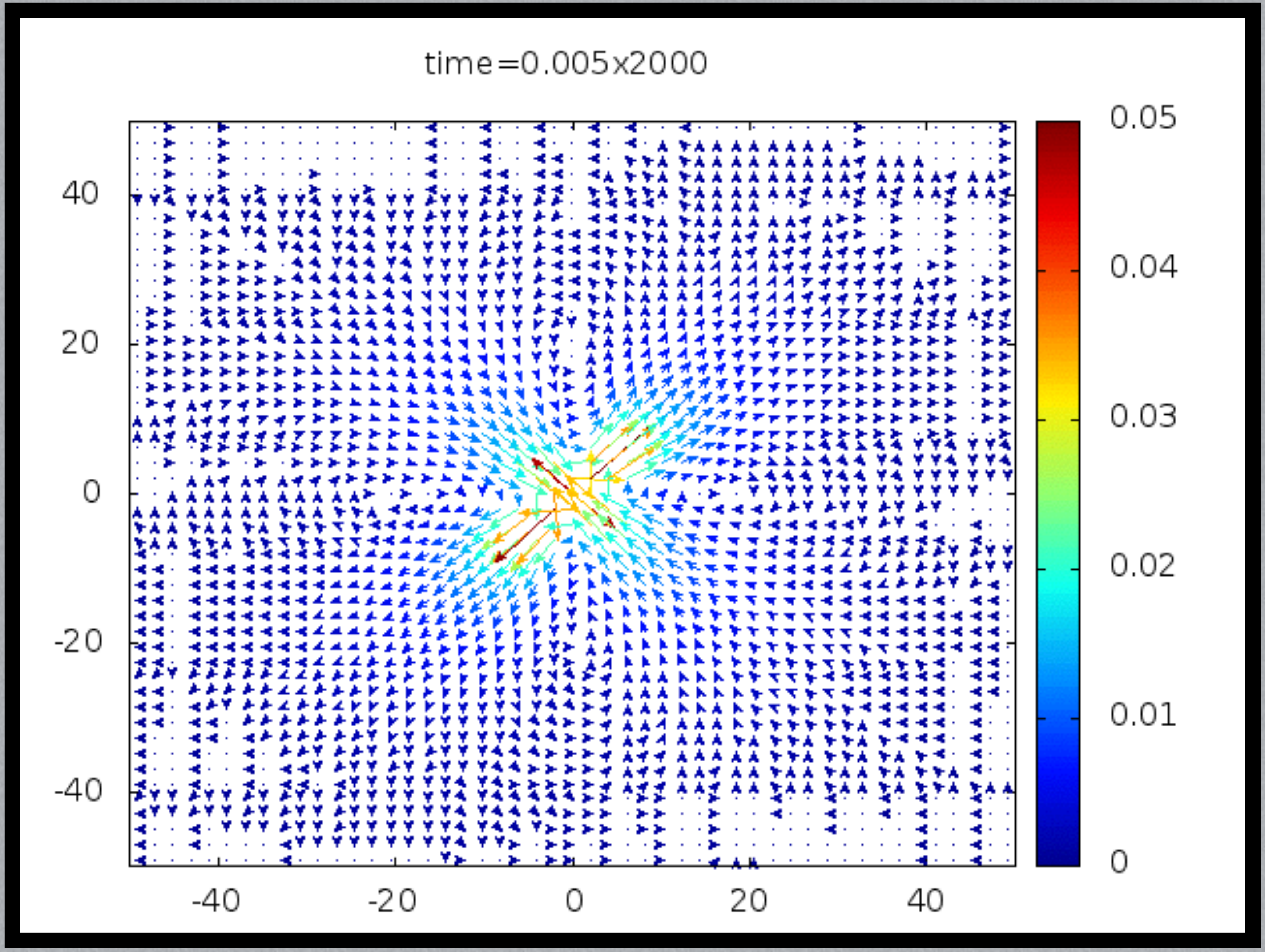
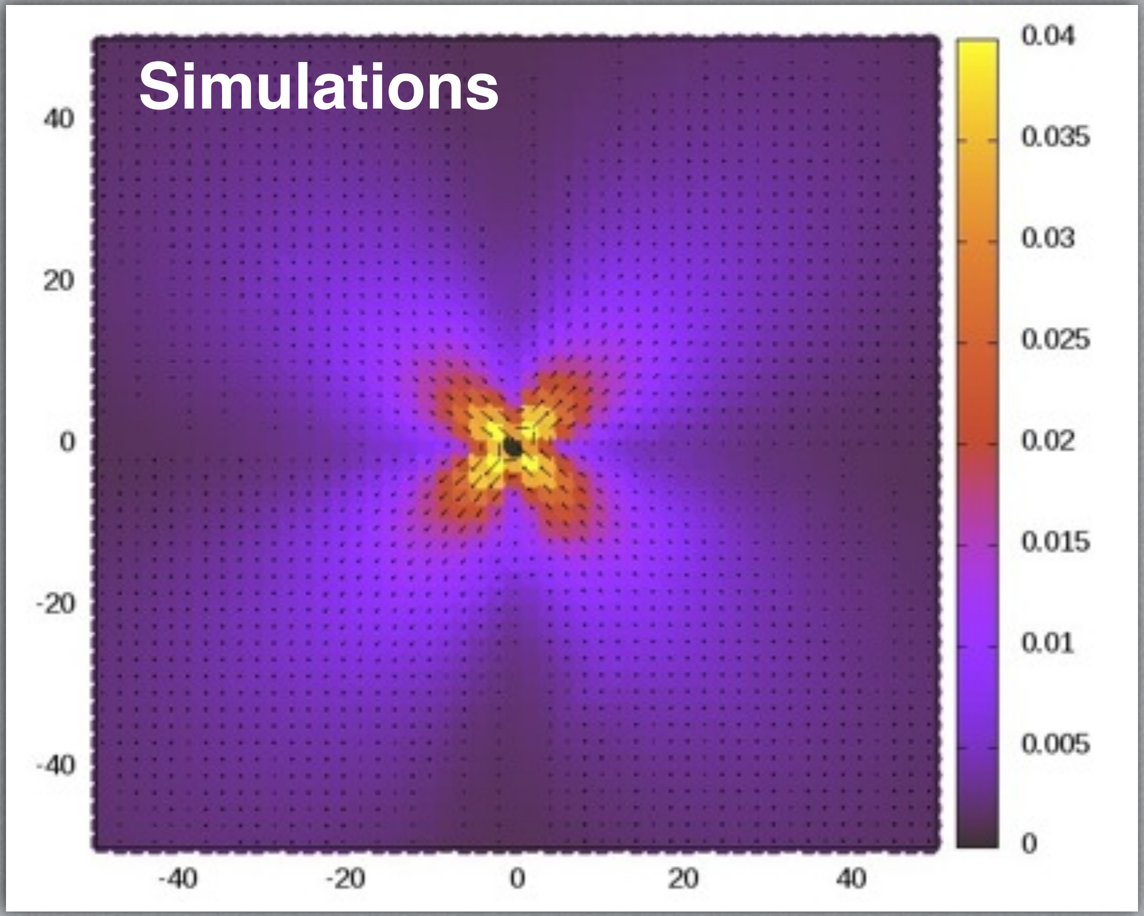
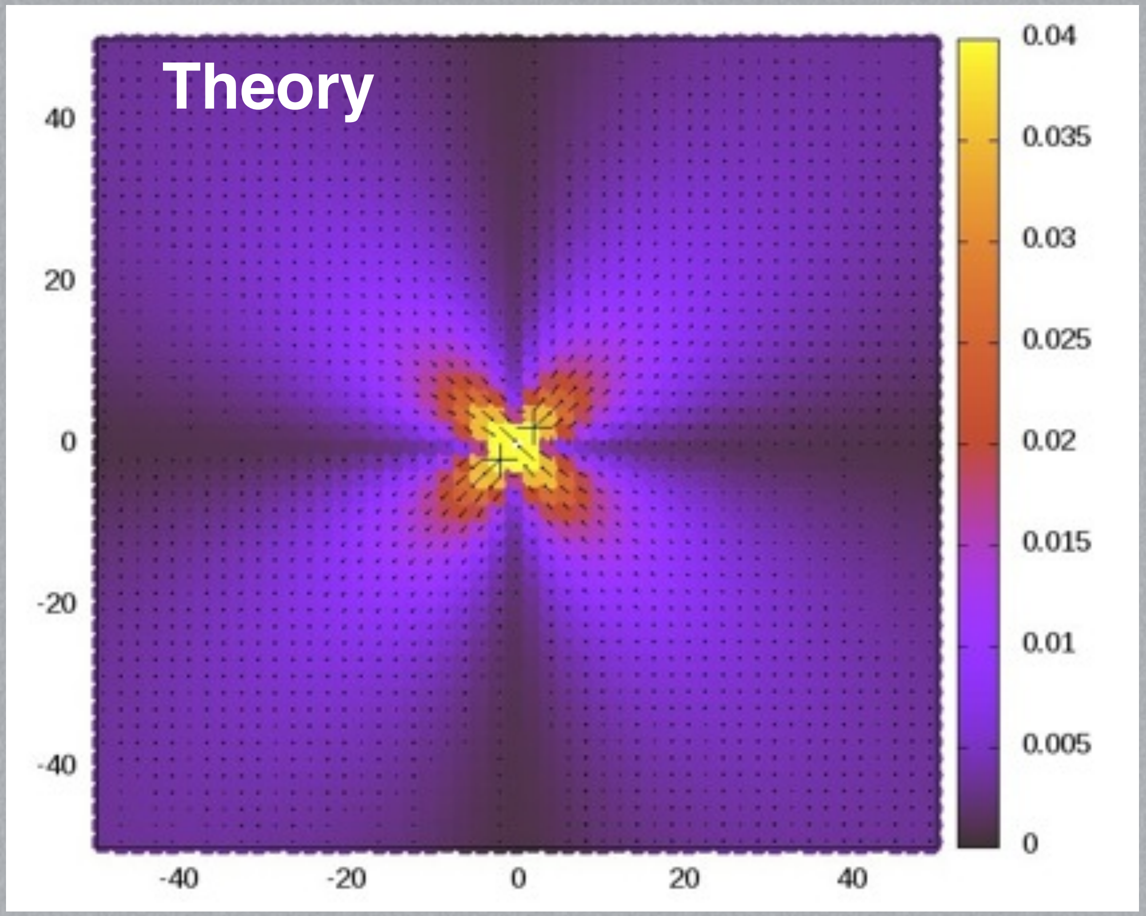


- **Average over disorder** by considering realizations of the ST in different positions of the system.

Equilibrium response: Eshelby theory





The long time equilibrium response averages out to the prediction of the Eshelby inclusion problem…

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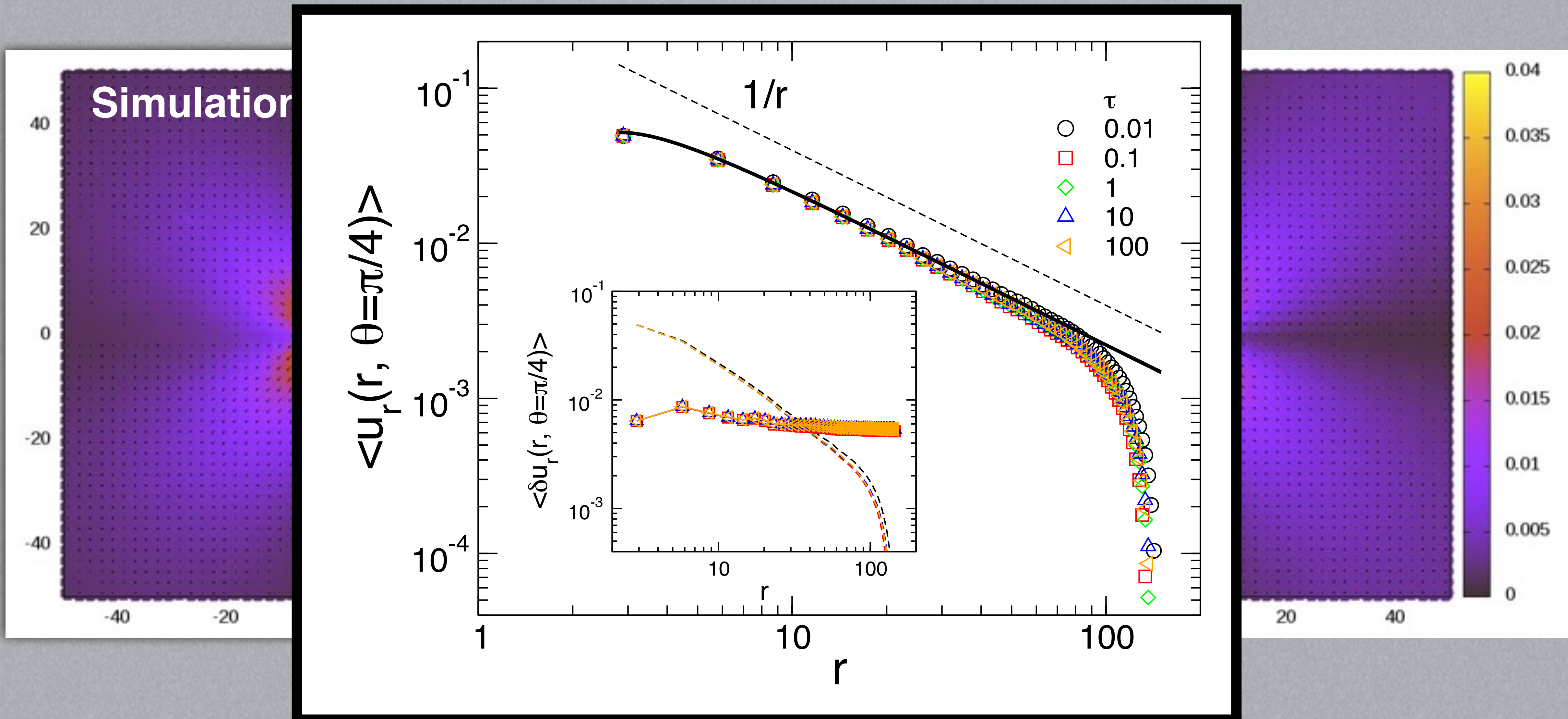


The long time equilibrium response averages out to the prediction of the Eshelby inclusion problem…

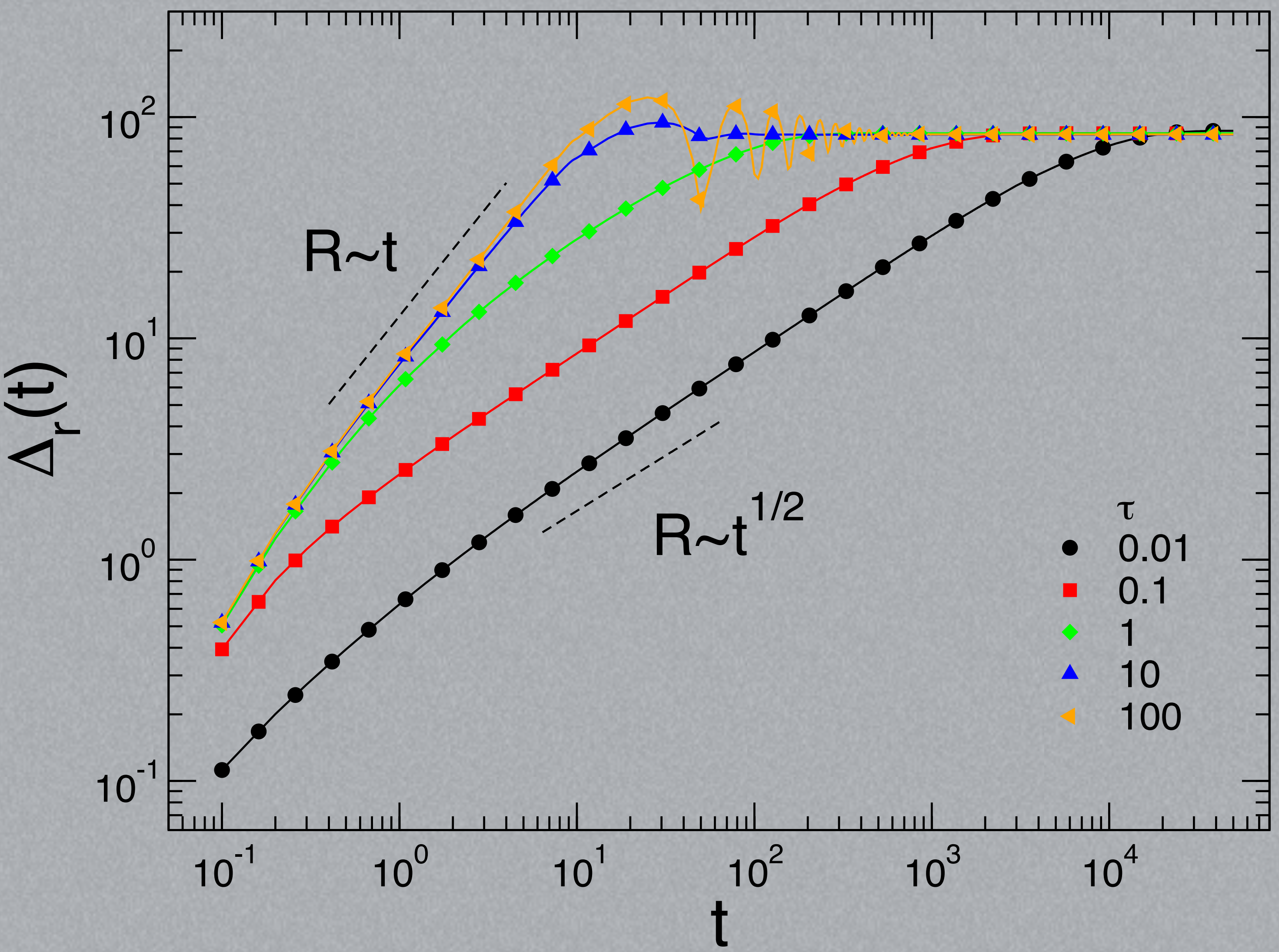
in spite of **very strong fluctuations**.

Propagation regime

total radial displacement $\Delta_r(t) = \int_{box} |\langle u_r(r,\theta,t)\rangle| d\mathbf{r}$

$$u_r(r,\theta,t) = u_r^{ce}(r,\theta)\Theta\left(r - R(t)\right) \Longrightarrow \Delta_r(t) \propto R(t)$$

R(t): estimate of the propagation distance



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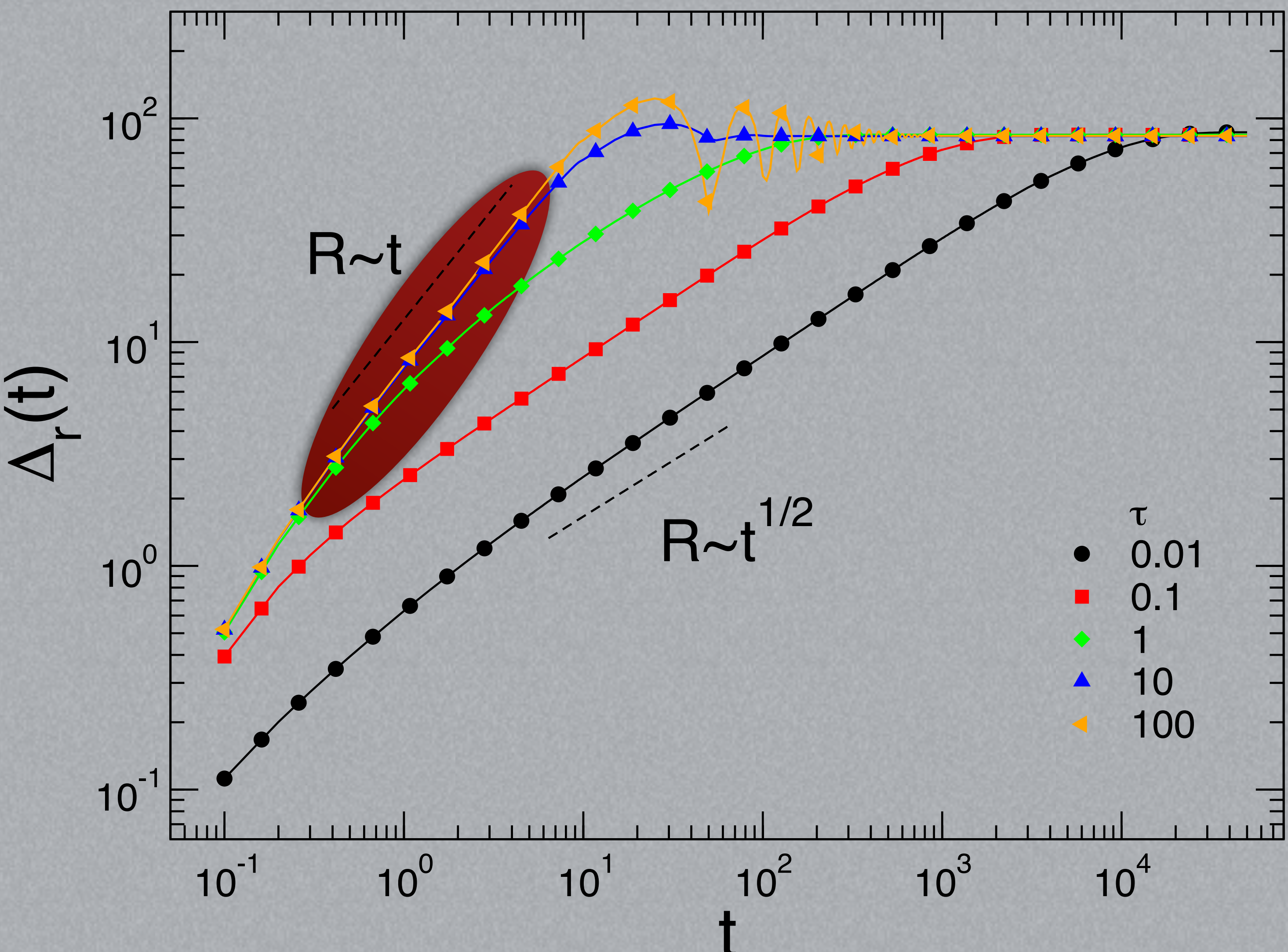

Underdamped dynamics

ballistic propagation

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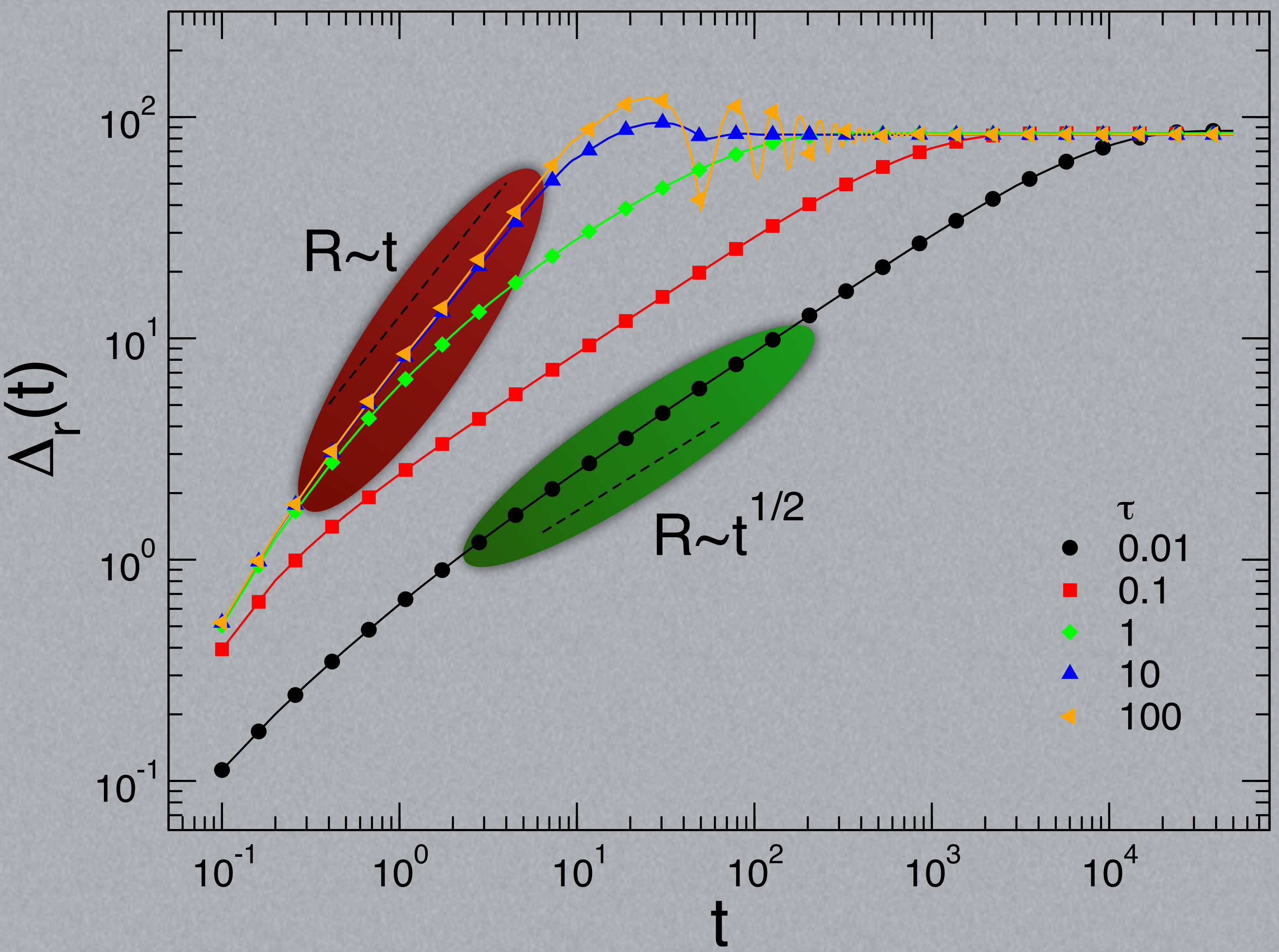


Underdamped dynamics

ballistic propagation

Overdamped dynamics

diffusive propagation

Continuum elasticity: time dependent solution

Diffusion equation for the displacement field:

$$\Gamma \frac{\partial u_\alpha}{\partial t} = \mu_2 \frac{\partial^2 u_\alpha}{\partial R_\beta \partial R_\beta} + \frac{\mu_2}{1-\nu_2} \frac{\partial^2 u_\beta}{\partial R_\alpha \partial R_\beta}$$

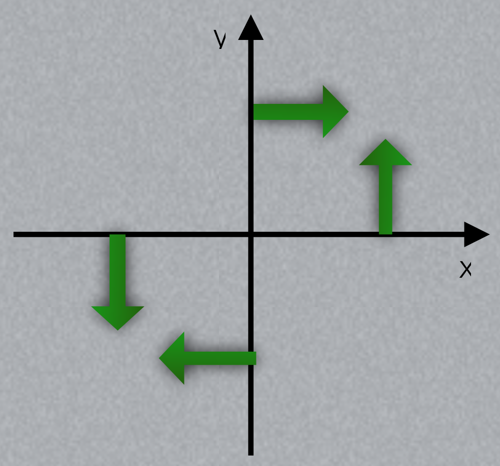
shear modulus: μ_2 Poisson ratio: ν_2

damping parameter: $\Gamma = \tau^{-1}$

Associated Green's tensor (Idema and Liu (2013)):

$$\begin{aligned} G_{ijk}(\mathbf{r},t) &= -\frac{1}{\mu_2 r}\left\{\left[\left(\frac{1-\nu_2}{2}+\frac{8D_2 t}{r^2}\right)e^{-r^2/4D_1 t} - \left(1+\frac{8D_2 t}{r^2}\right)e^{-r^2/4D_2 t}\right]\frac{r_i r_j r_k}{r^3}\right. \\ &- \left.\frac{2D_2 t}{r^2}\left[e^{-r^2/4D_1 t} - e^{-r^2/4D_2 t}\right]\phi_{ijk} + \delta_{ik}\frac{r_j}{r}e^{-r^2/4D_2 t}\right\} \end{aligned}$$

D1, D2: longitudinal and transverse diffusion coefficients



Perturbation due to a set of force dipoles of magnitude:

$P = a^2 \mu \epsilon^*$

(Picard et al (2004))

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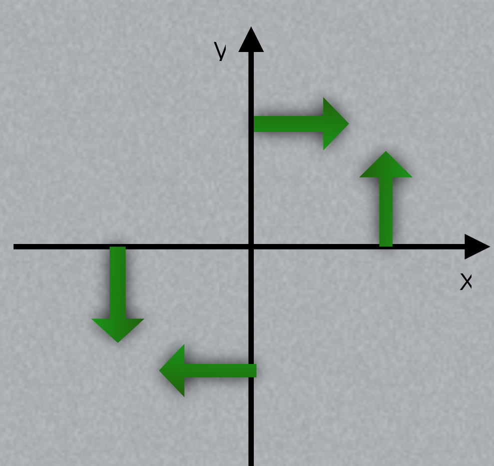

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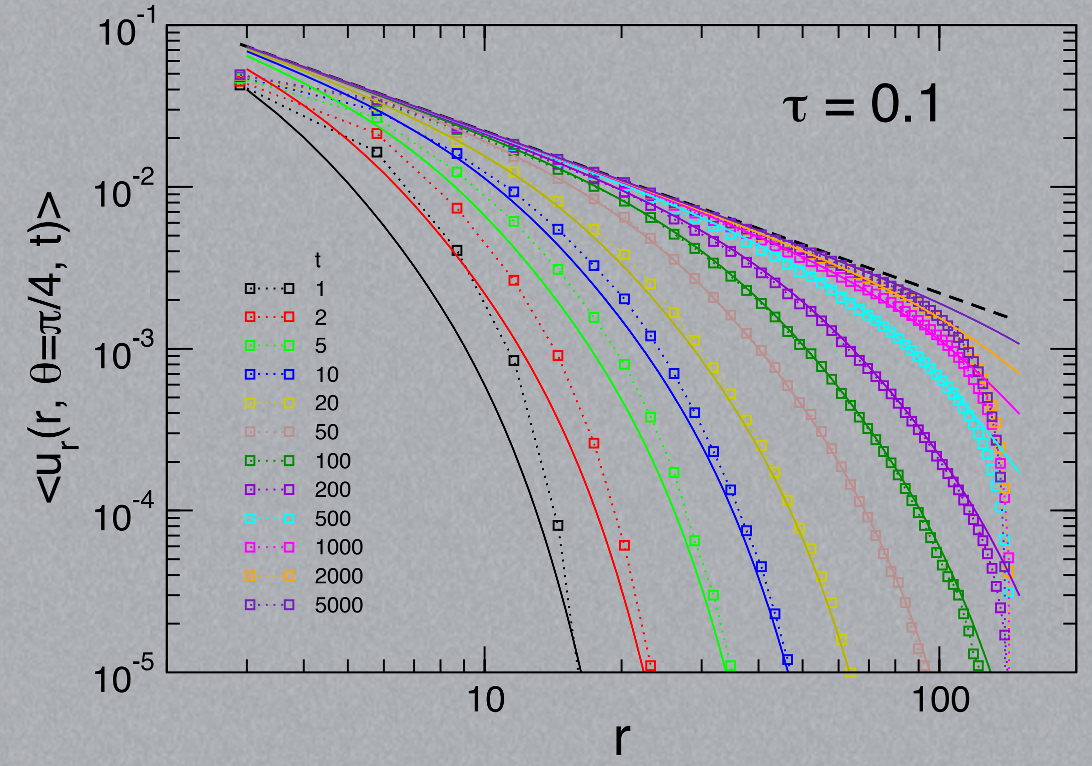

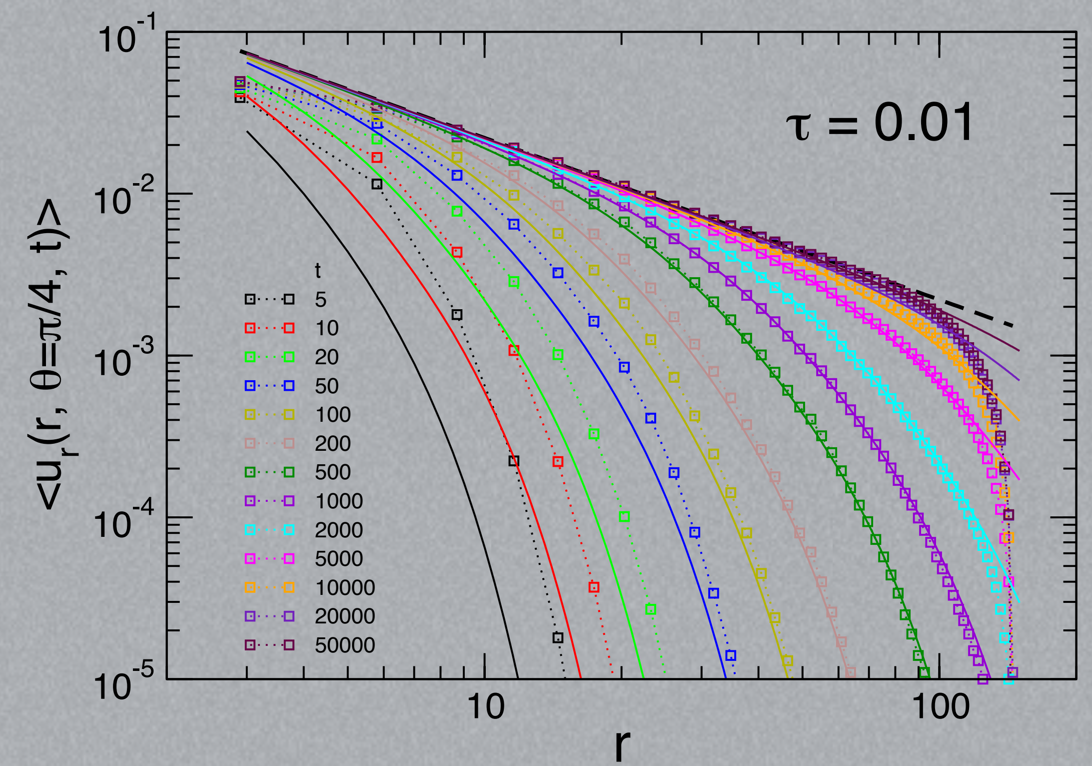

Large strain: plastic activity

Indicator of **plasticity**: deviations from an affine deformation on a local scale;
locally, around particle *i,* the minimum over all possible linear deformation tensors of

$$D^2(i;t,\delta t) = \sum_j \left[r_{ij}(t+\delta t) - (\mathbb{I}+\epsilon)\cdot r_{ij}(t)\right]$$

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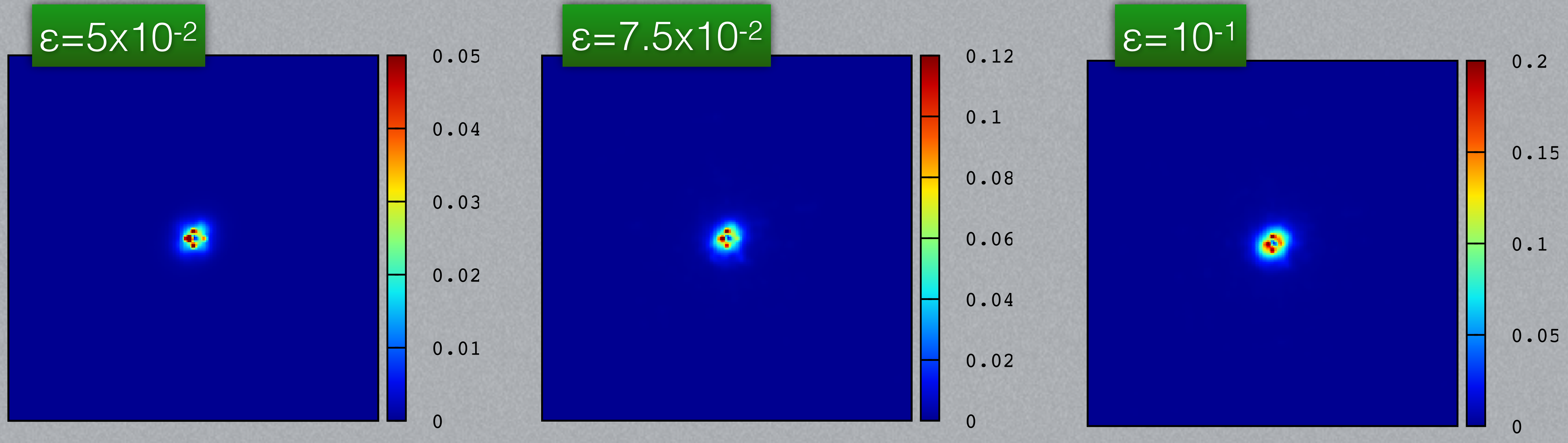

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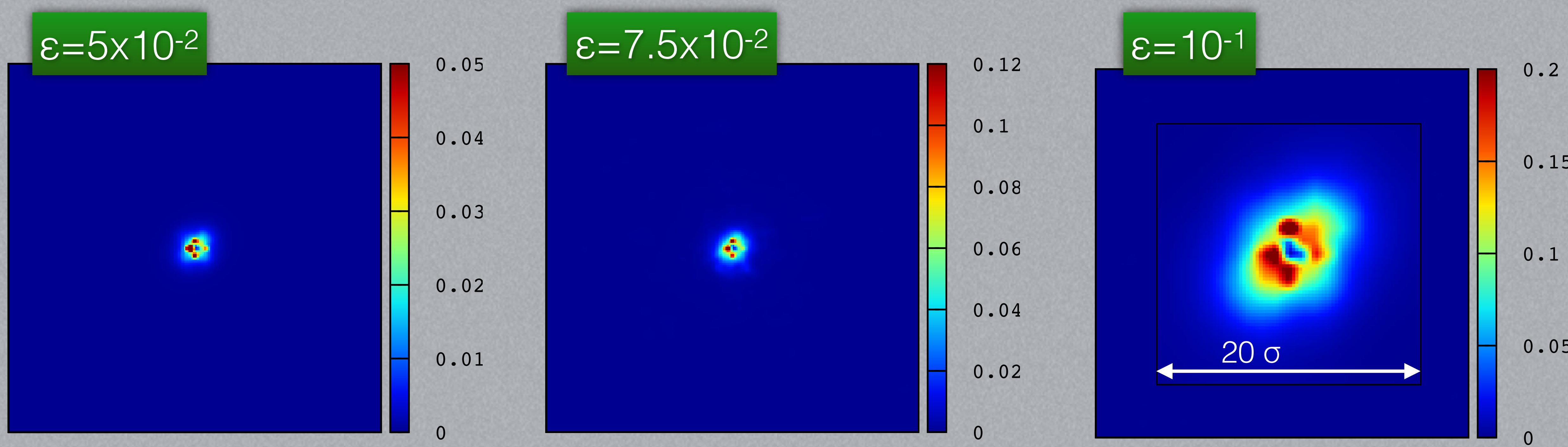
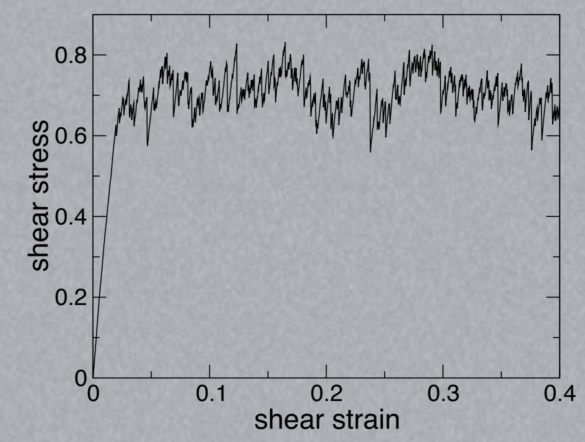


Very **weak** plastic effects, **localized** in the vicinity of the ST.

Plasticity in presheared systems

The system is sheared at a rate 10^{-6} by deforming the box dimensions and remapping the particle positions.

Configurations are extracted at random strain values in the steady state.



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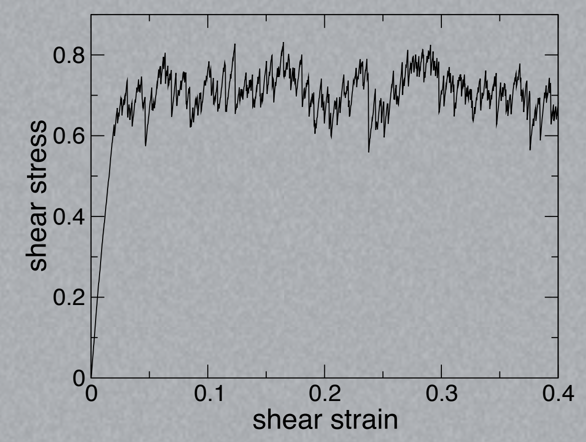
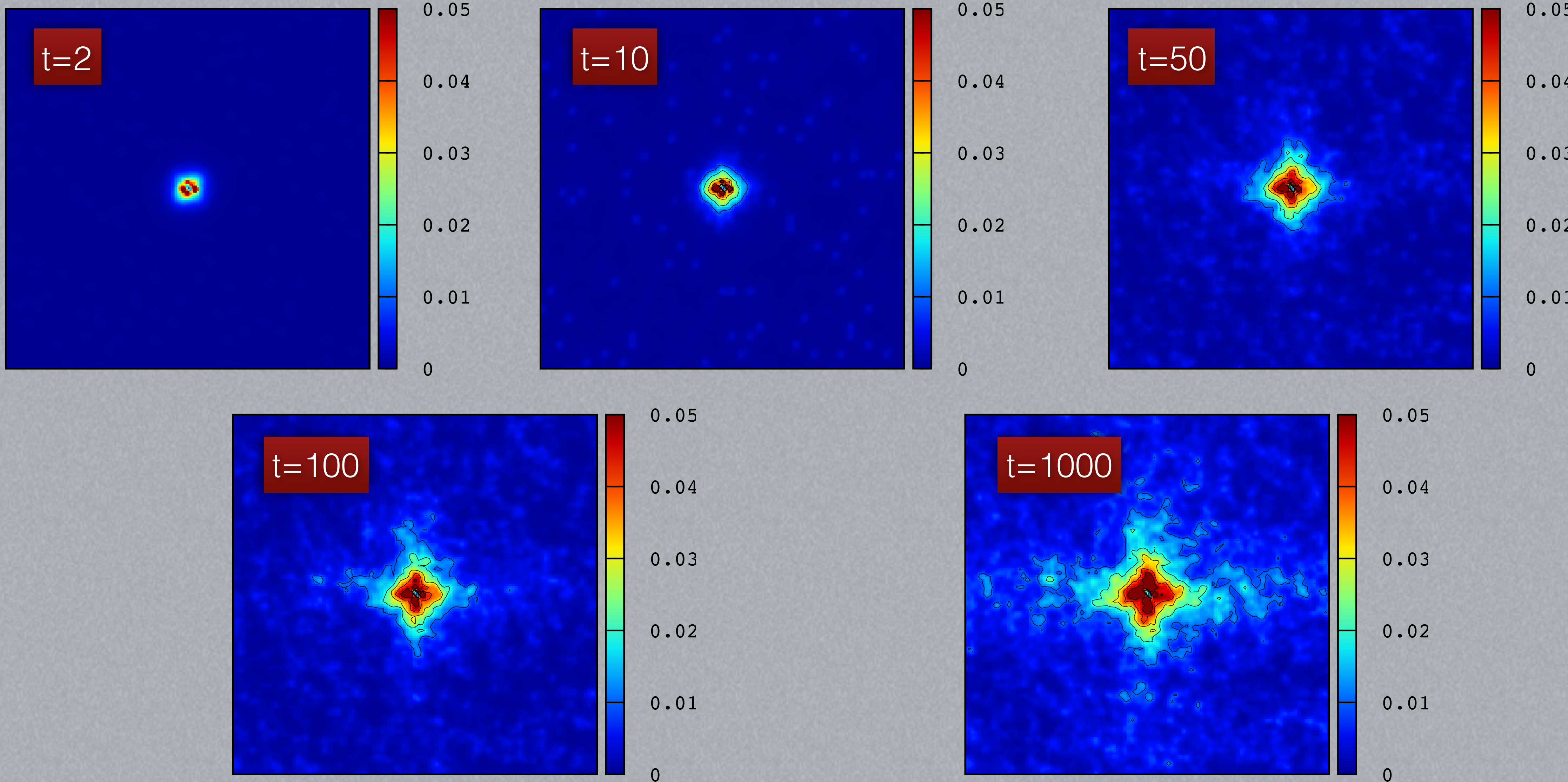
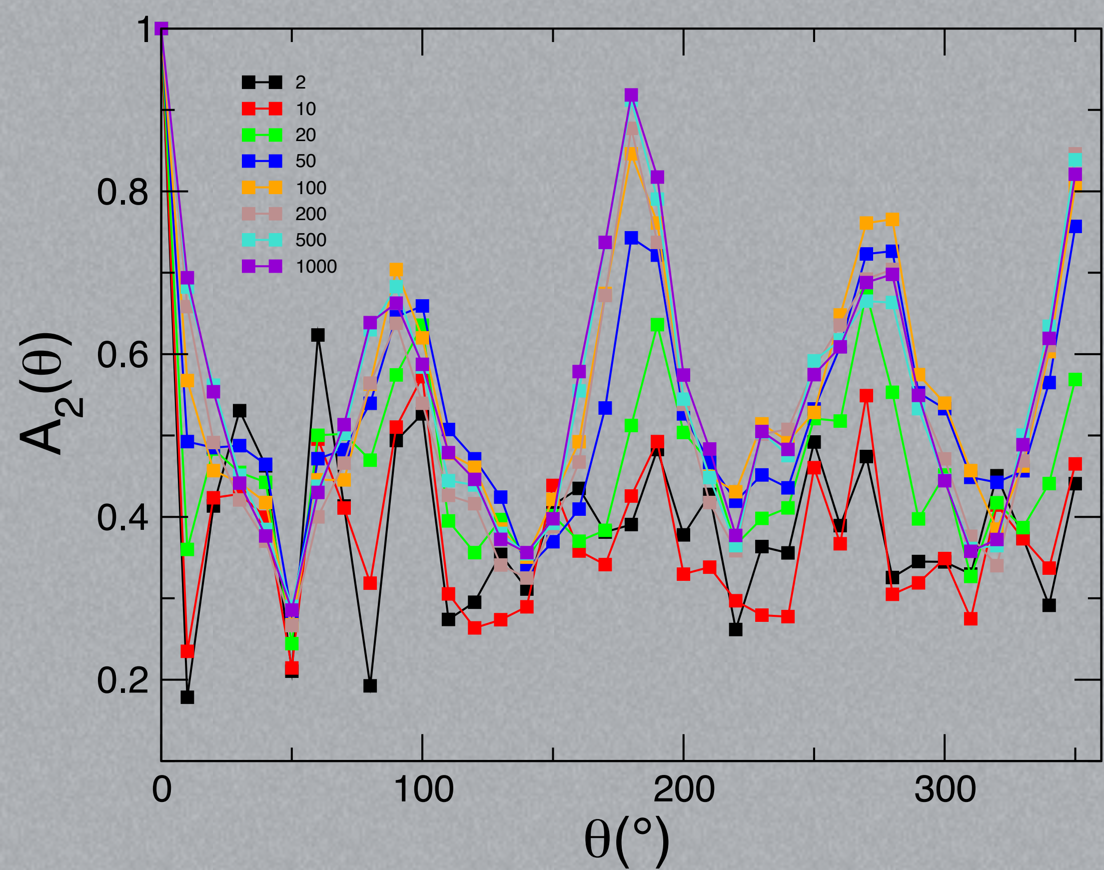




Plastic correlations

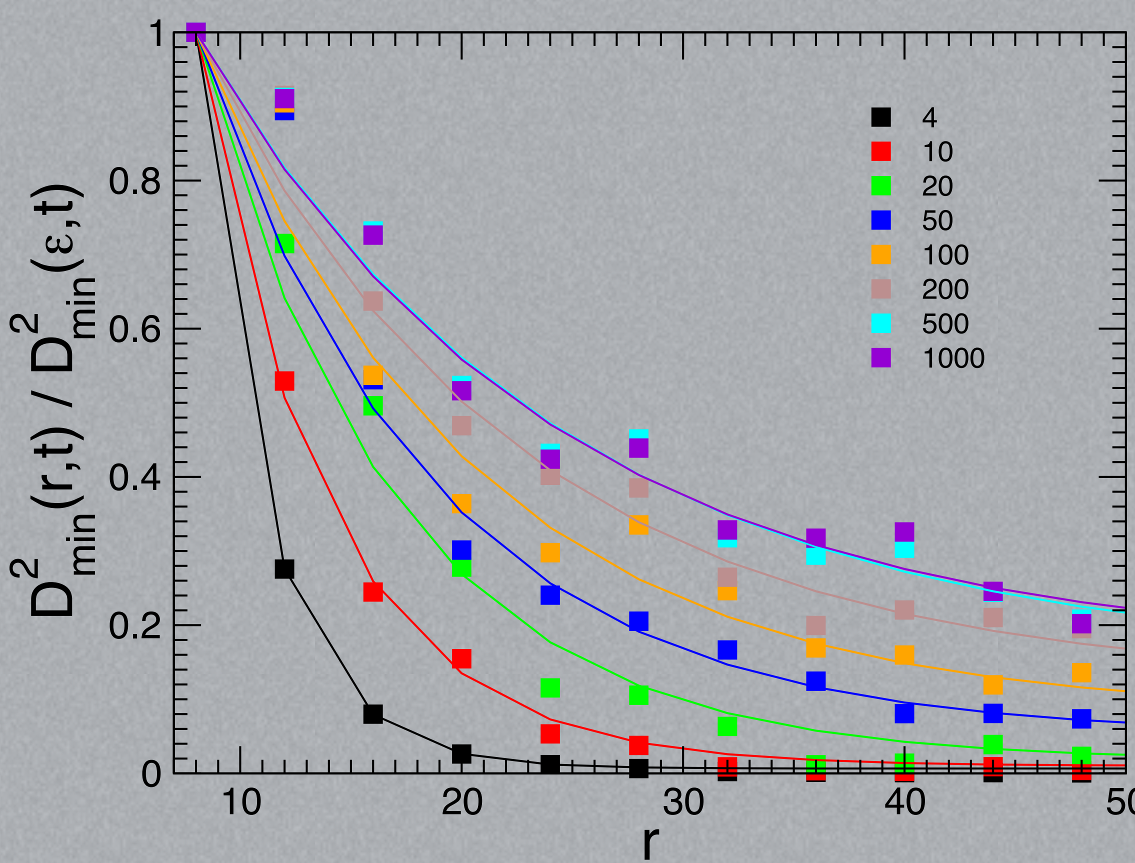
Angular dependence of the plastic activity

$$A_2(\theta, t) = \alpha \int_0^{L/2} D^2_{min}(r, \theta, t) dr$$



Asymmetry of the streamwise and crosswise lobes, also observed in spatiotemporal correlations between plastic events in flowing systems (Nicolas et al (2014)).

Spatial decay of the correlations in the flow directions



Exponential decay, due to the mean-field frictional force in the equation of motion (Varnik et al (2014)).

Summary

- Despite large fluctuations, the equilibrium response to a ST average out to the prediction of Eshelby inclusion problem for a continuum elastic medium.

- We characterize the effect of inertia on the propagation of an elastic signal: a crossover from propagative transmission in the case of underdamped dynamics to a diffusive transmission for overdamped is evidenced.

- In the overdamped case the full time-dependent elastic response is in good agreement with the theoretical predictions.

- Plastic effects in presheared configurations are in qualitative agreement with the observations of plastic correlations in sheared glasses.

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