Stochastic approach to non-affine deformations in jammed granular packing

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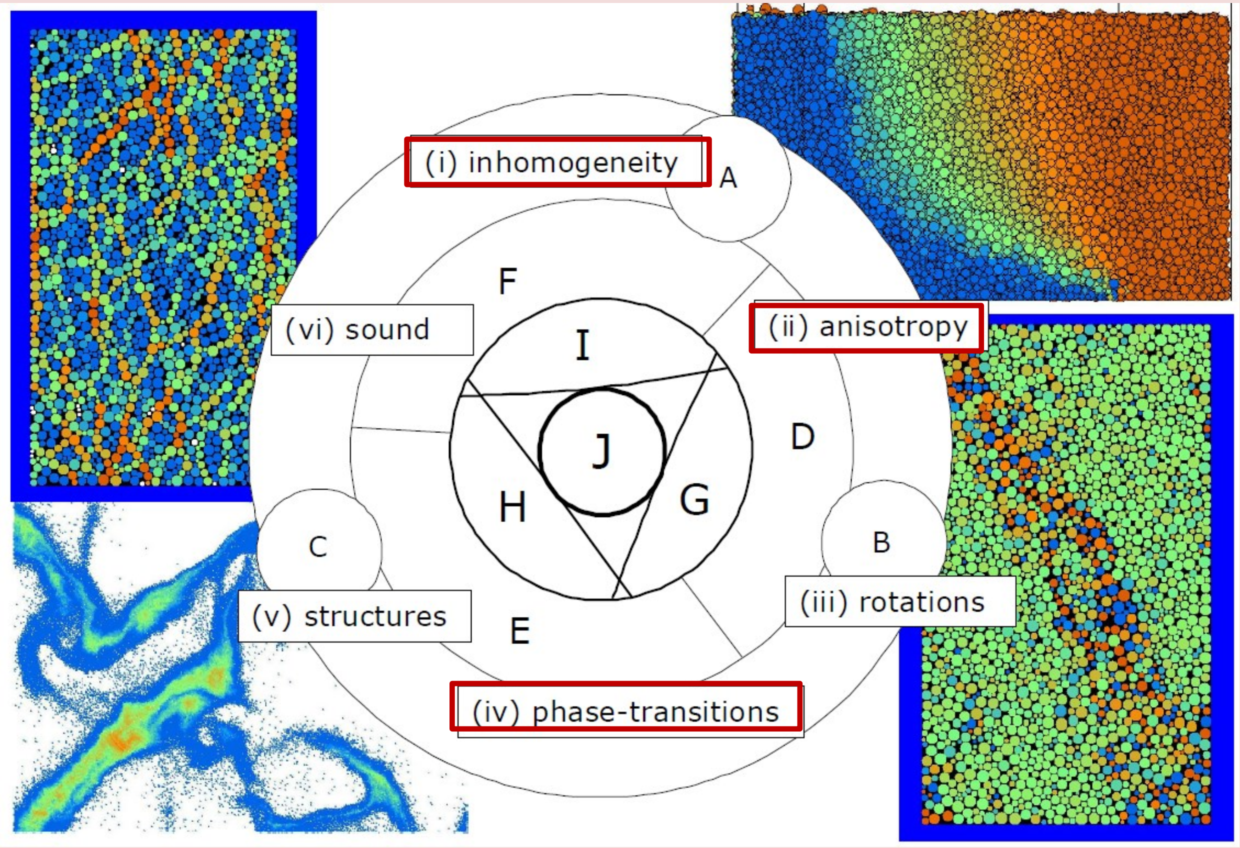
Aim

"Bridging the gap between particulate systems and continuum theory"

- Vici project, No. 10828

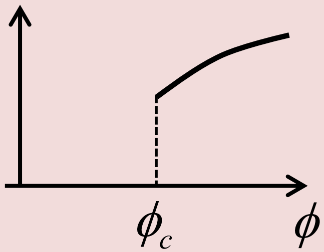


Non-affine responses of granular assemblies to global deformations

Background

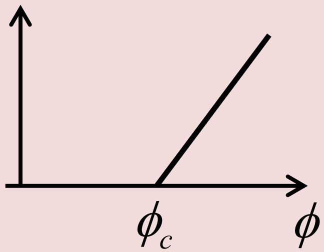
Jamming – analogy with critical phenomena

coordination number



the 1st order like

static pressure



the 2nd order like

Granular particles are *out of equilibrium*
due to *the dissipation of energy* and *absence of temperature*

[O'Hern, L. E. Silbert, A. J. Liu, and S. R. Nagel, PRE **68** (2003) 011306]

Statistical mechanics

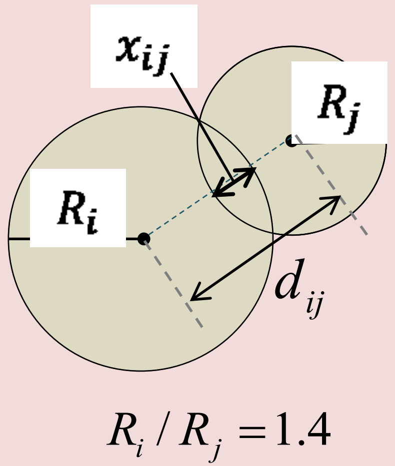
Edward's ensembles, force ensembles, etc.

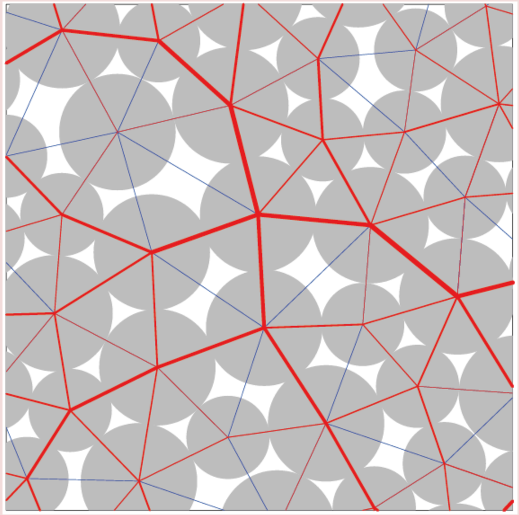
[Edwards & Oakeshott (1989), Henkes & Chakraborty (2009), Tighe, Snoeijer, et. al. (2010)]

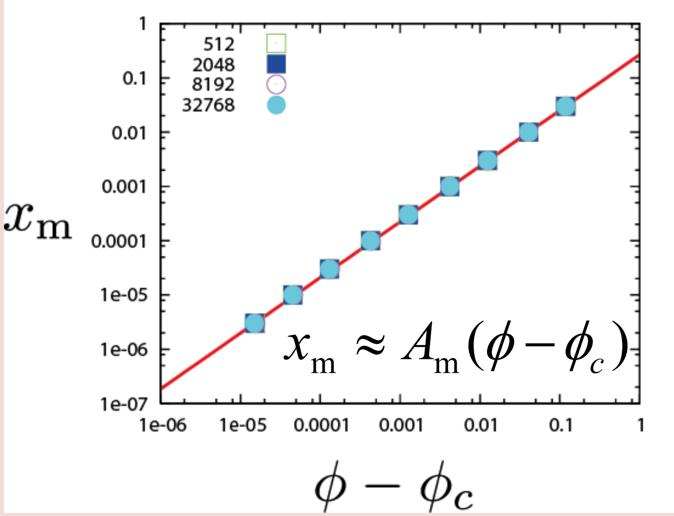
Statistical weight, i.e. probability distribution functions (PDFs) of forces

We take a different approach to the "granular statistical mechanics" to describe the PDFs under global deformations.

Method







Molecular dynamics simulations

Binary mixtures of 2D frictionless particles (50:50) filled in a square periodic box

Contact force $f_{ij} = -kx_{ij} - \eta \dot{x}_{ij}$

Global damping $\mathbf{f}_i = -\eta \mathbf{v}_i$

System size & samples

N=512, 2048, and 8192 (10 samples), and N=32768 (2 samples)

Static packings

We adjust the diameters by controlling the mean overlap over all particles x_m

unjammed $x_m = 0$ *jammed* $x_m > 0$

Non-affine response

Isotropic compression

Rescaling every radius

$$R_i \rightarrow \sqrt{1+\frac{\delta\phi}{\phi}}R_i$$

$$\phi \rightarrow \phi + \delta\phi$$

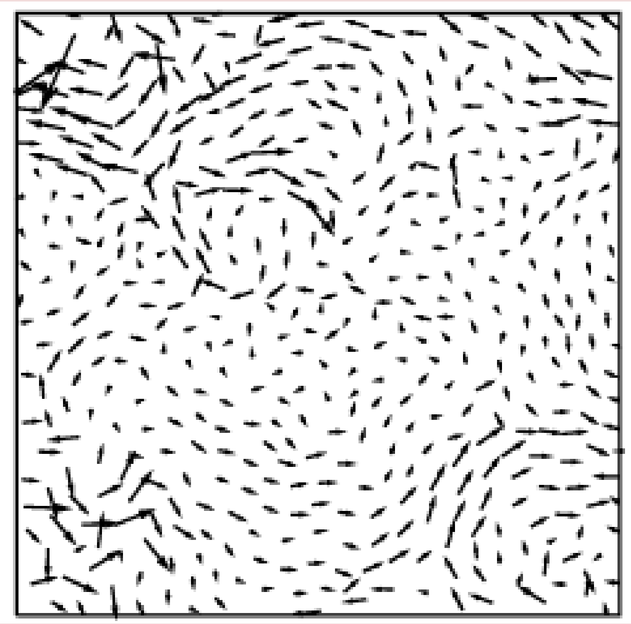
Affine response (*immediately after compression*)

$$x^{\mathrm{affine}}(\phi+\delta\phi) = x(\phi) + (d/2\phi)\delta\phi$$

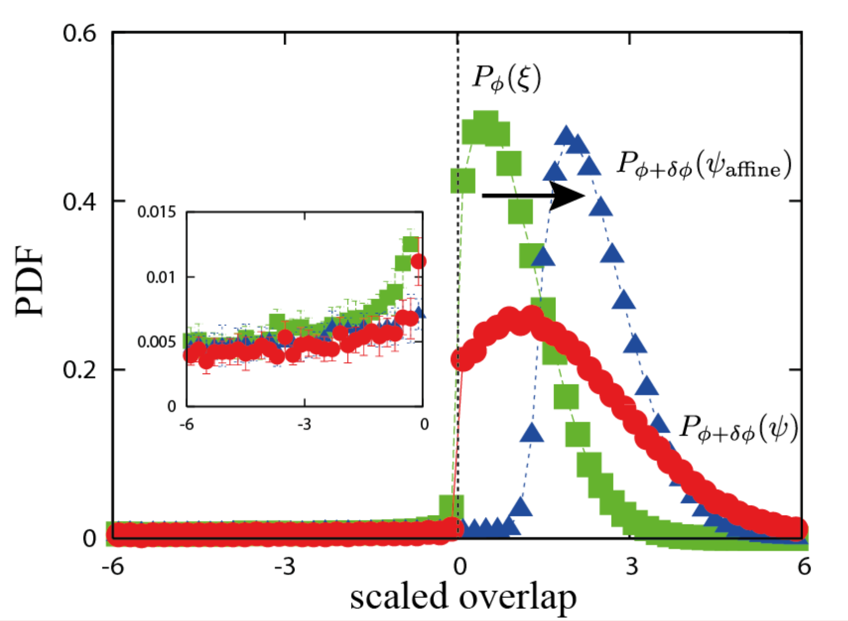
Non-affine response (*after relaxation*)

$$x(\phi+\delta\phi) \neq x^{\mathrm{affine}}(\phi+\delta\phi)$$

Displacements of particles

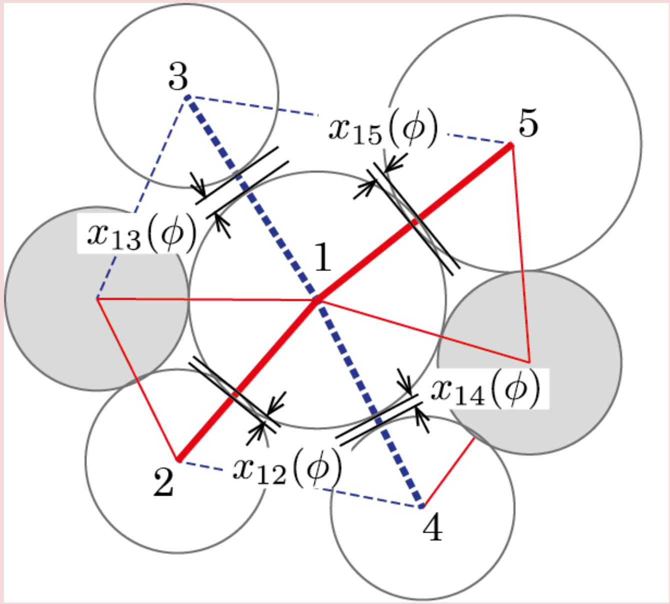


PDFs of overlaps

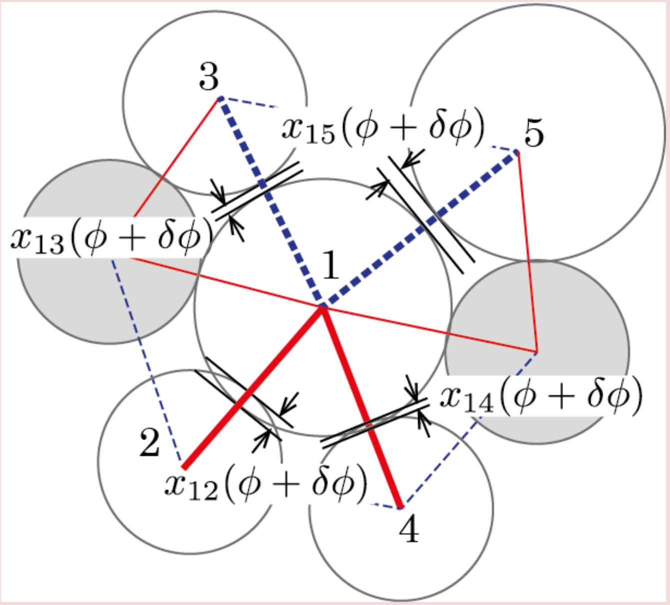


Microscopic insights

Before compression



After relaxation



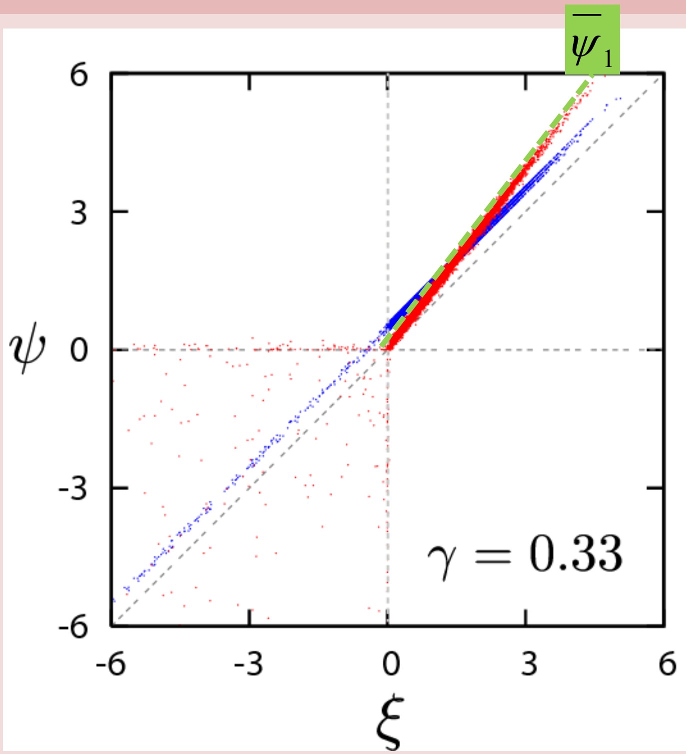
Contact-to-contact (CC) $x_{12}(\phi) > 0 \rightarrow x_{12}(\phi+\delta\phi) > 0$

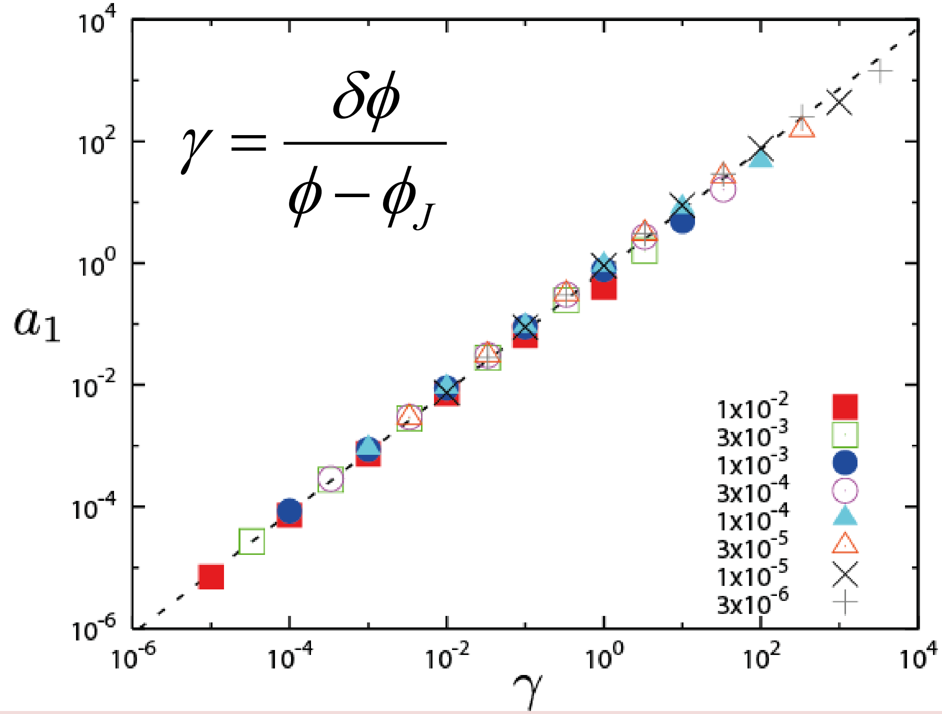
Virtual-to-virtual (VV) $x_{13}(\phi) < 0 \rightarrow x_{13}(\phi+\delta\phi) < 0$

Virtual-to-contact (VC) = *"closing contact"* $x_{14}(\phi) < 0 \rightarrow x_{14}(\phi+\delta\phi) > 0$

Contact-to-virtual (CV) = *"opening contact"* $x_{15}(\phi) > 0 \rightarrow x_{15}(\phi+\delta\phi) < 0$

Power law scaling





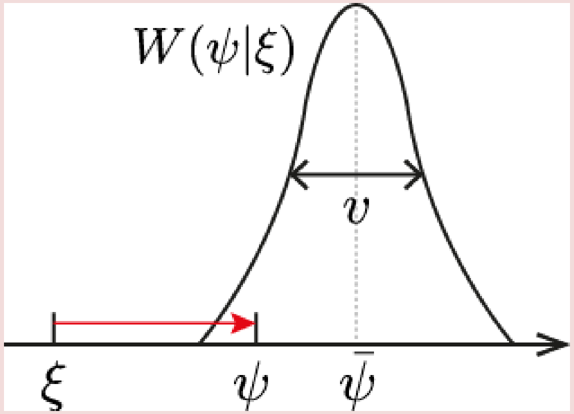
Mean	$\overline{\psi}_1(\xi) = (a_1 + 1)\xi + b_1$
Excess slope	$a_1 = A_1\gamma$
Offsets	$b_1,\ \ b_2 \ \sim\ \gamma$
Standard deviations	$v_1,\ \ v_2 \ \sim\ \gamma$

Degree of non-affinity increases with γ

Stochastic approach

*Affine response => **deterministic***

*Non-affine response => **stochastic***



Conditional probability distribution

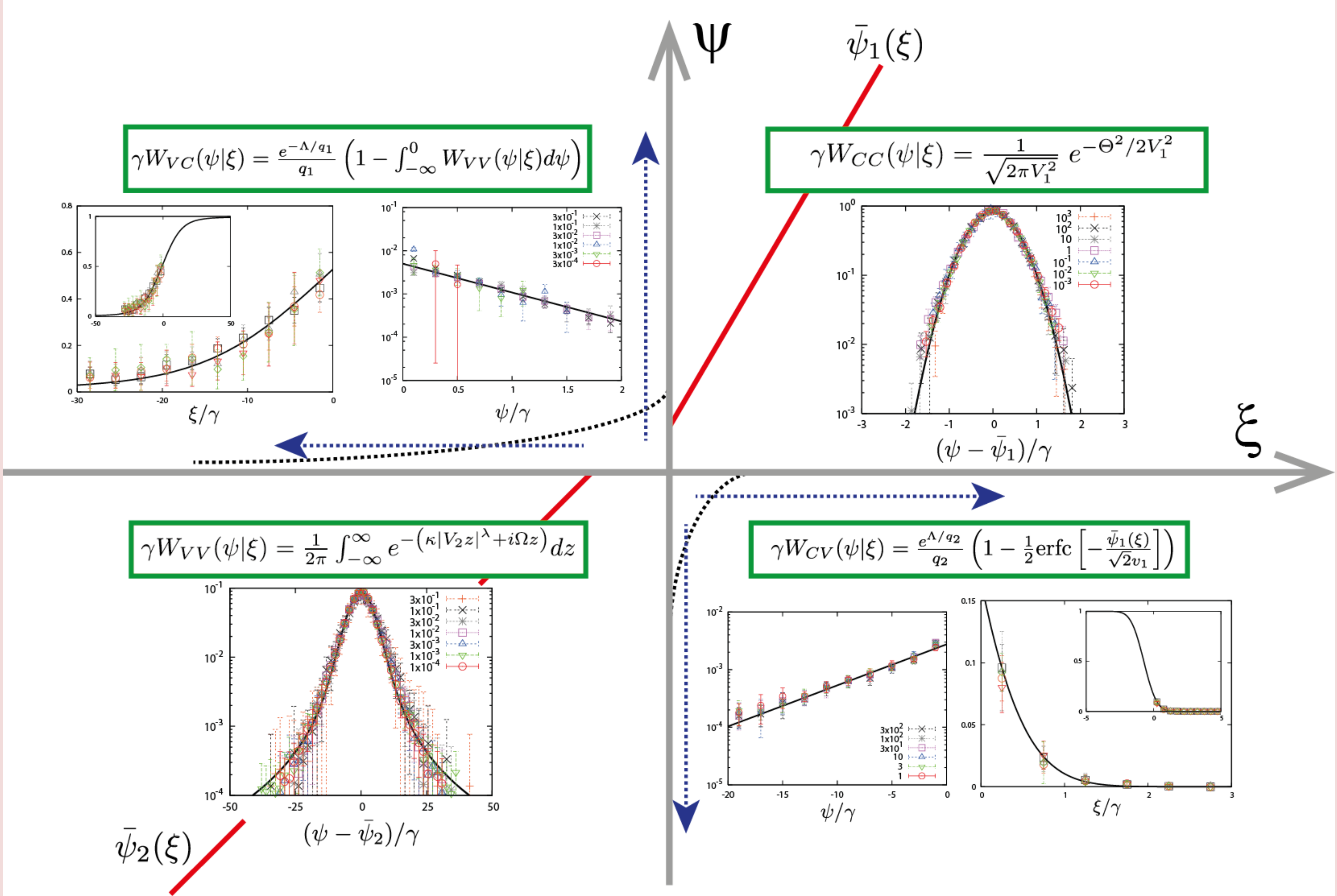
$$P_{\phi+\delta\phi}(\psi) = \int_{-\infty}^{\infty} W(\psi \mid \xi) P_{\phi}(\xi)\, d\xi$$

Transition rate $T(\psi \mid \xi) = W(\psi \mid \xi)/\delta\phi$

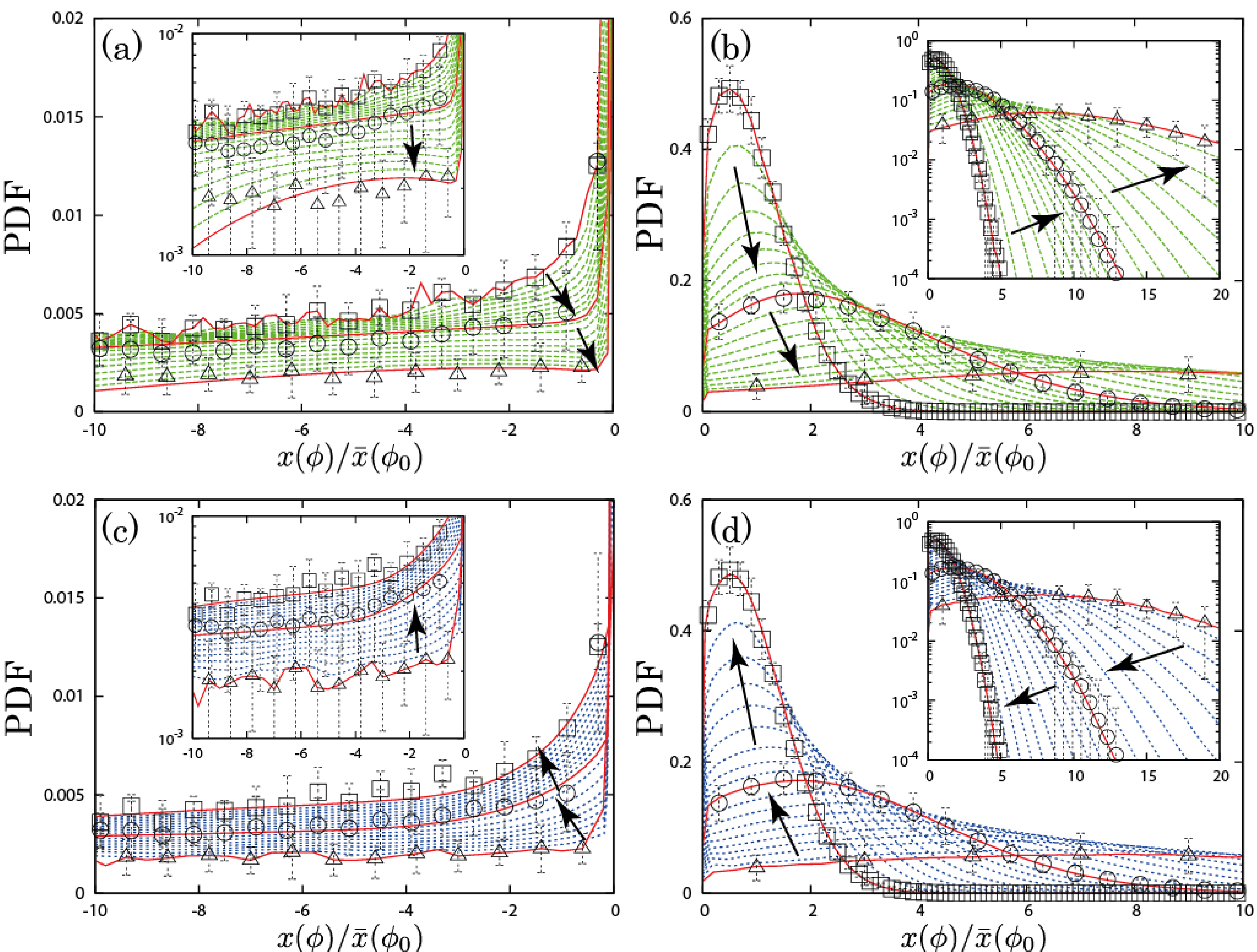
Master equation

$$\frac{\partial}{\partial \phi} P_{\phi}(\psi) = \int_{-\infty}^{\infty} \left[T(\psi \mid \xi) P_{\phi}(\xi) - T(\xi \mid \psi) P_{\phi}(\psi)\right] d\xi$$

Conditional probability distributions



Master equation



Moments

The n-th "moment"

$$M_n = \int_0^\infty x^n P_\phi(x)\, dx$$

coordination number

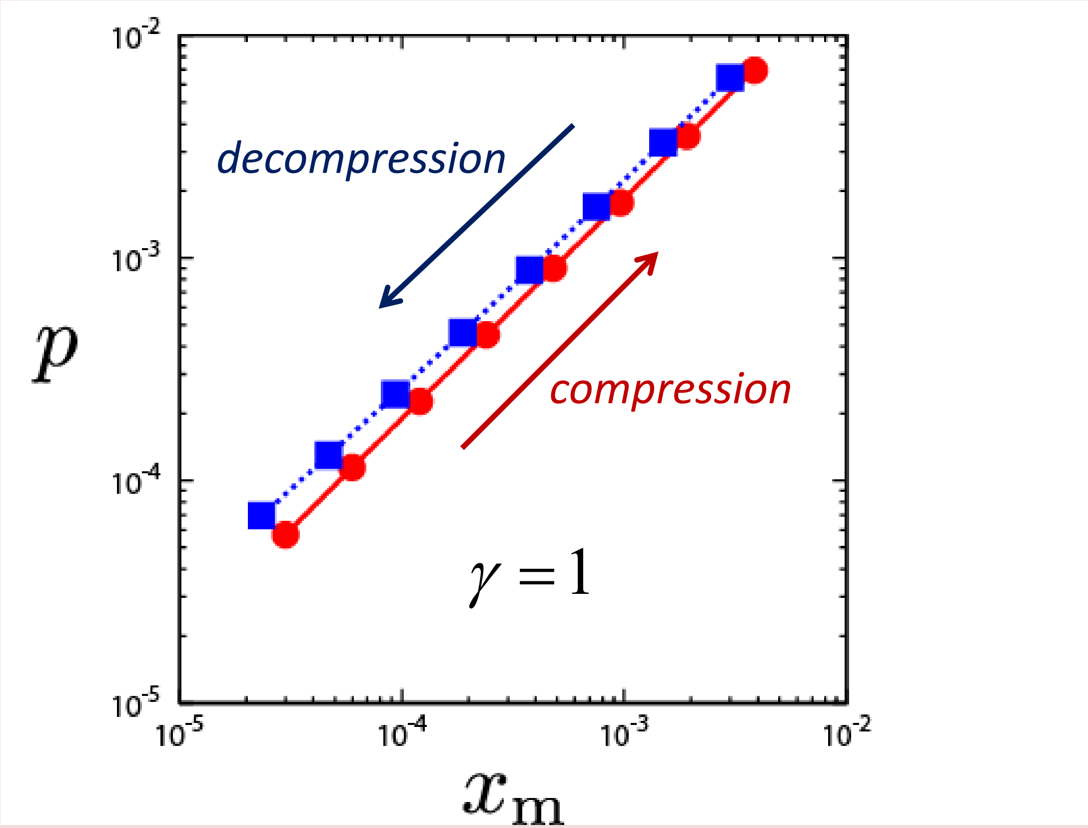
$$z \propto M_0$$

mean overlap

$$x_m \propto M_1$$

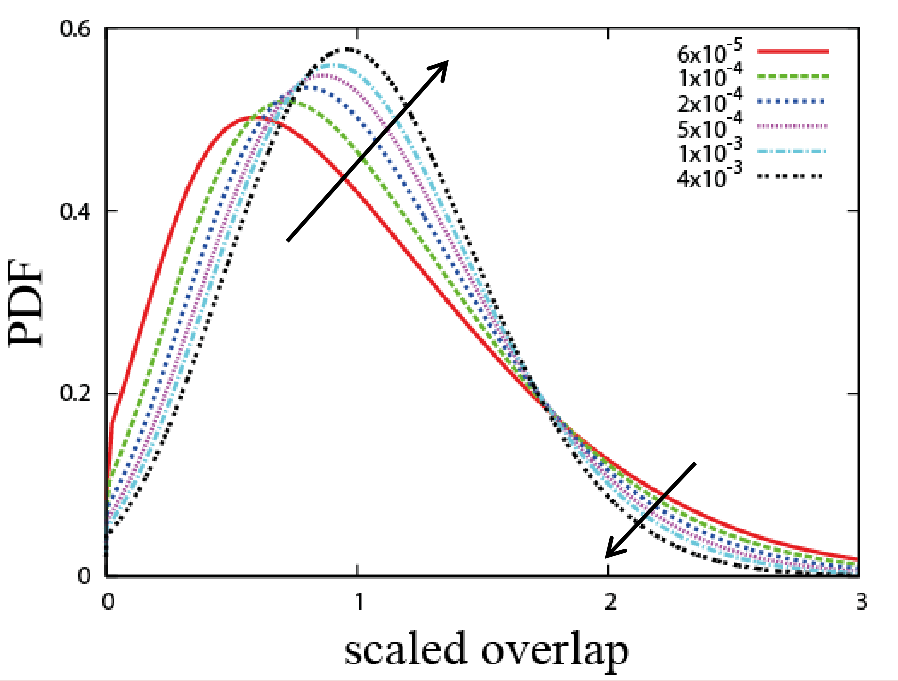
static pressure

$$p \propto \bar{\sigma} M_1 - M_2$$

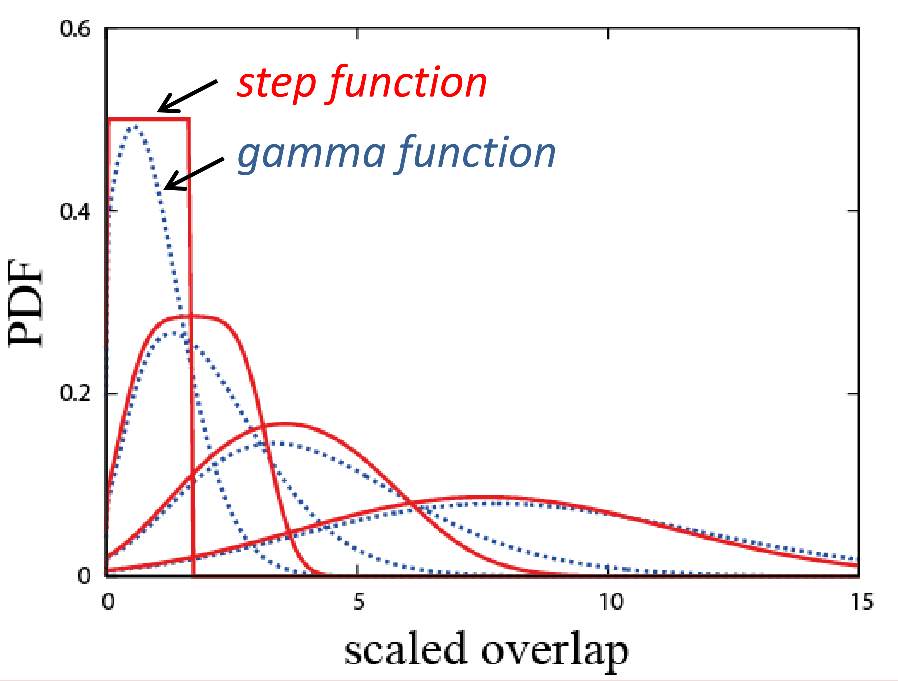


Applications

Shape analysis

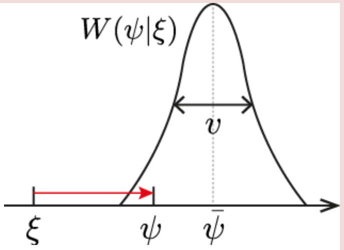


Dependence on initial conditions



Stochastic model

Stochastic model for a single overlap



$$x(\phi+\delta\phi) = \boxed{\text{Mean}} + \boxed{\text{Fluctuation}}$$

$$= \left[A_1\,\delta\phi/(\phi-\phi_J)+1\right]x(\phi) + A_{\mathrm{m}}(1-A_1)\delta\phi + \zeta_1\delta\phi$$

$$\therefore \boxed{\frac{dx}{d\phi} = \frac{A_1}{\phi-\phi_J}x(\phi) + A_{\mathrm{m}}(1-A_1) + \zeta_1 \qquad (x>0)}$$

Analogue to the Langevin equation

The distribution of the noise is a Gaussian, i.e. white noise, with the width $V_1\delta\phi$

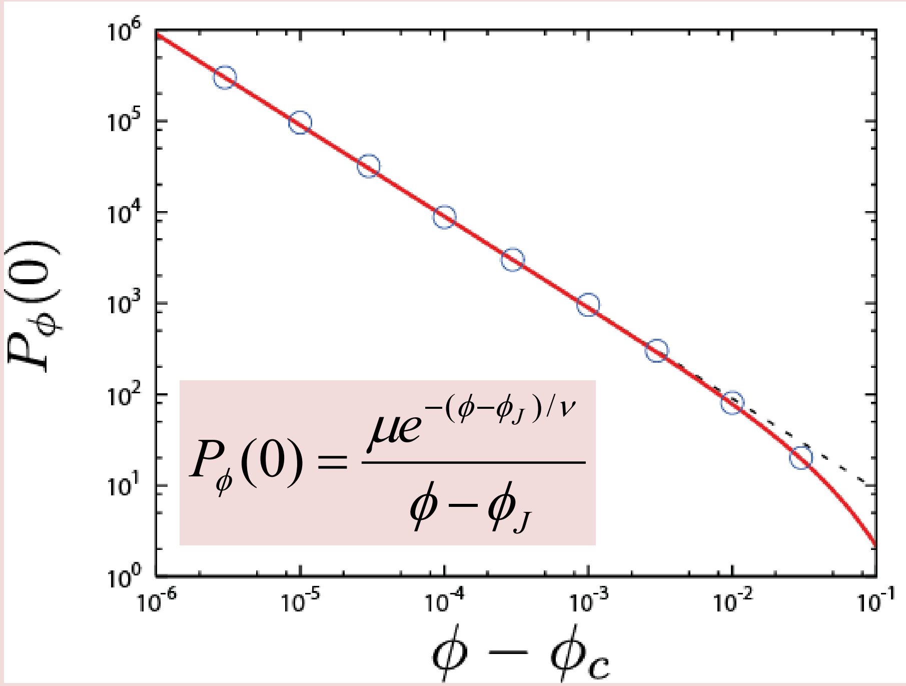
The Fokker-Planck equation

$$\frac{\partial}{\partial\phi}P_\phi(x) = \frac{(A_{\mathrm{m}}V_1)^2}{2}\frac{\partial^2}{\partial x^2}P_\phi(x) - \frac{\partial}{\partial x}\left[\alpha(x)P_\phi(x)\right]$$

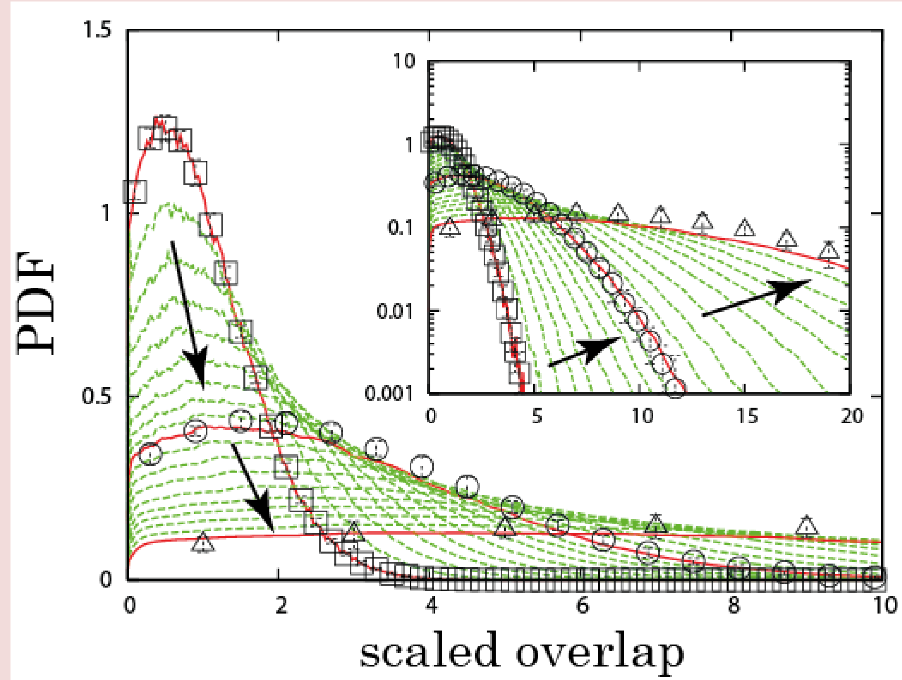
$$\alpha(x) \equiv \frac{A_1}{\phi-\phi_J}x + (1-A_1)A_{\mathrm{m}}$$

Fokker-Planck equation

Boundary condition



Numerical solutions



Initial condition the PDF with $\phi_0 - \phi_J = 4.0\times10^{-3}$

Increment of area fraction $\delta\phi = 10^{-5}$

Summary

- ✓ We take a *stochastic approach* to the non-affine responses of overlaps.
- ✓ The degree of *non-affinity* is linearly scaled by the ratio $\gamma = \dfrac{\delta\phi}{\phi - \phi_J}$
- ✓ *Conditional probability distributions* of overlaps are measured.
- ✓ *The master equation* well describes the PDFs under (de)compressions.
- ✓ We propose a *stochastic model* for a single overlap.
- ✓ *The Fokker-Planck equation* also works well.

Outlook ❑ Response to *shear*