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Introduction

- Granular media are vital in a diverse array of industries (e.g. agriculture, mining, and pharmaceutical manufacturing), and their behaviour is important in a variety of natural geophysical phenomena.
- In recent years, granular chains have been the focus of a number of studies¹ since they provide a simple, tractable model for more realistic systems and have numerous applications, ranging from vibration reduction and shock absorption² to detecting buried objects³, as well as energy harvesting and energy localization⁴.
- In general, any velocity perturbation to an end grain in an uncompressed 1D granular chain will propagate through the system as a nondispersive bundle of energy, or solitary wave (SW)⁵.
- SWs in the granular chain are not preserved in collisions with other SWs or boundaries. Rather, the SW breaks up and reforms in the collision process, resulting in the partial destruction of the initial SW and the birth of secondary solitary waves (SSWs).
- A sufficiently long time after an initial perturbation to the system, rates of breakdown and creation processes of SSWs balance and the chain reaches a steady state called the *quasi-equilibrium* (QEQ) phase⁶.
- Here we investigate how the system's journey to QEQ can be tuned by varying the material parameters of the granular chain system, and the effects of introducing an inertial mismatch at the boundary on the onset and rate of relaxation to the QEQ phase.
- We subsequently analyze the extreme long-term behaviour of these granular systems.

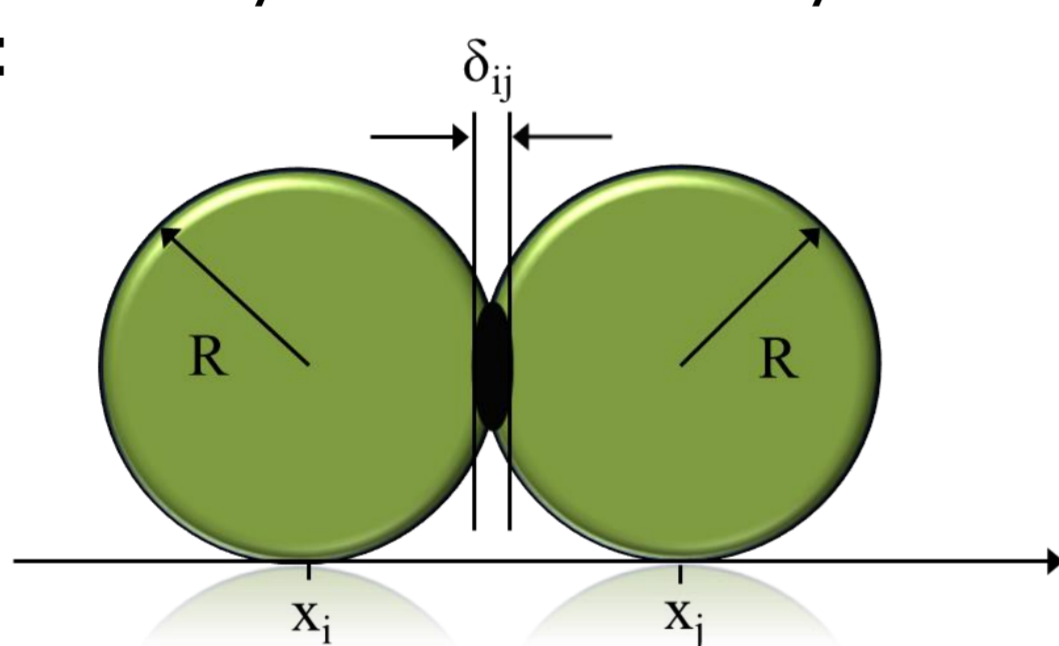
Methods

- Grains interact only when they are in physical contact, and the interaction is governed by the intrinsically nonlinear Hertz potential⁷:

$$V(\delta_{ij}) = A_{ij} \delta_{ij}^{5/2}$$

$$A_{ij} = \frac{2}{5D_{ij}} \sqrt{\frac{R_i R_j}{R_i + R_j}}$$

$$D_{ij} = \frac{3}{4} \left[\frac{1 - \sigma_i^2}{Y_i} + \frac{1 - \sigma_j^2}{Y_j} \right]$$



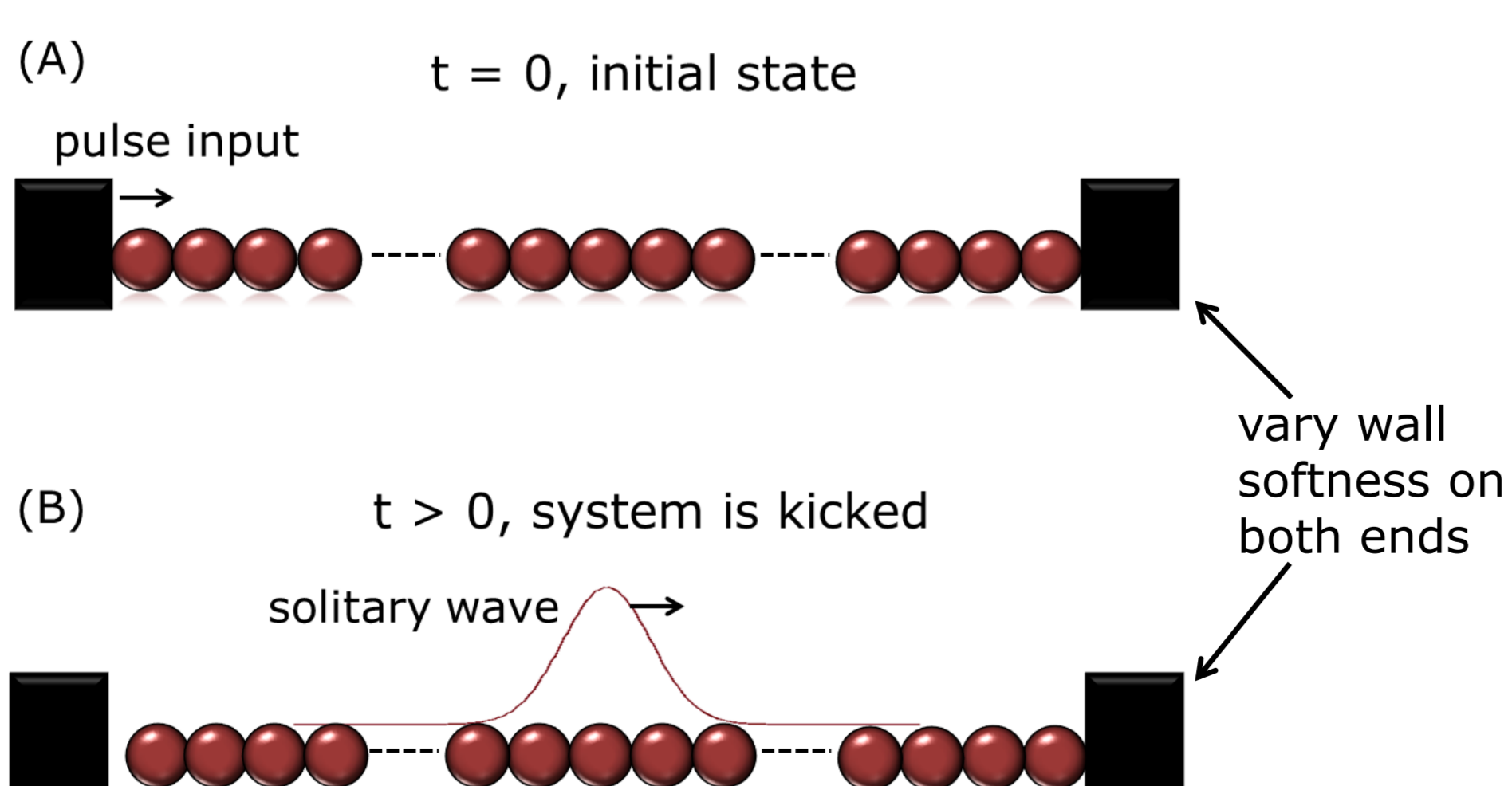
$$\delta_{ij} = 2R - (x_j - x_i) \geq 0$$

$$\delta_{ij} = u_i - u_j \geq 0$$

- Equations of motion for any non-edge grain in the chain are then given by

$$m_i \ddot{u}_i = \frac{5}{2} \left(A_{i-1,i} (u_{i-1} - u_i)^{3/2} - A_{i,i+1} (u_i - u_{i+1})^{3/2} \right)$$

- A typical simulation involves perturbing an uncompressed, monodispersed granular chain held between fixed symmetric walls:

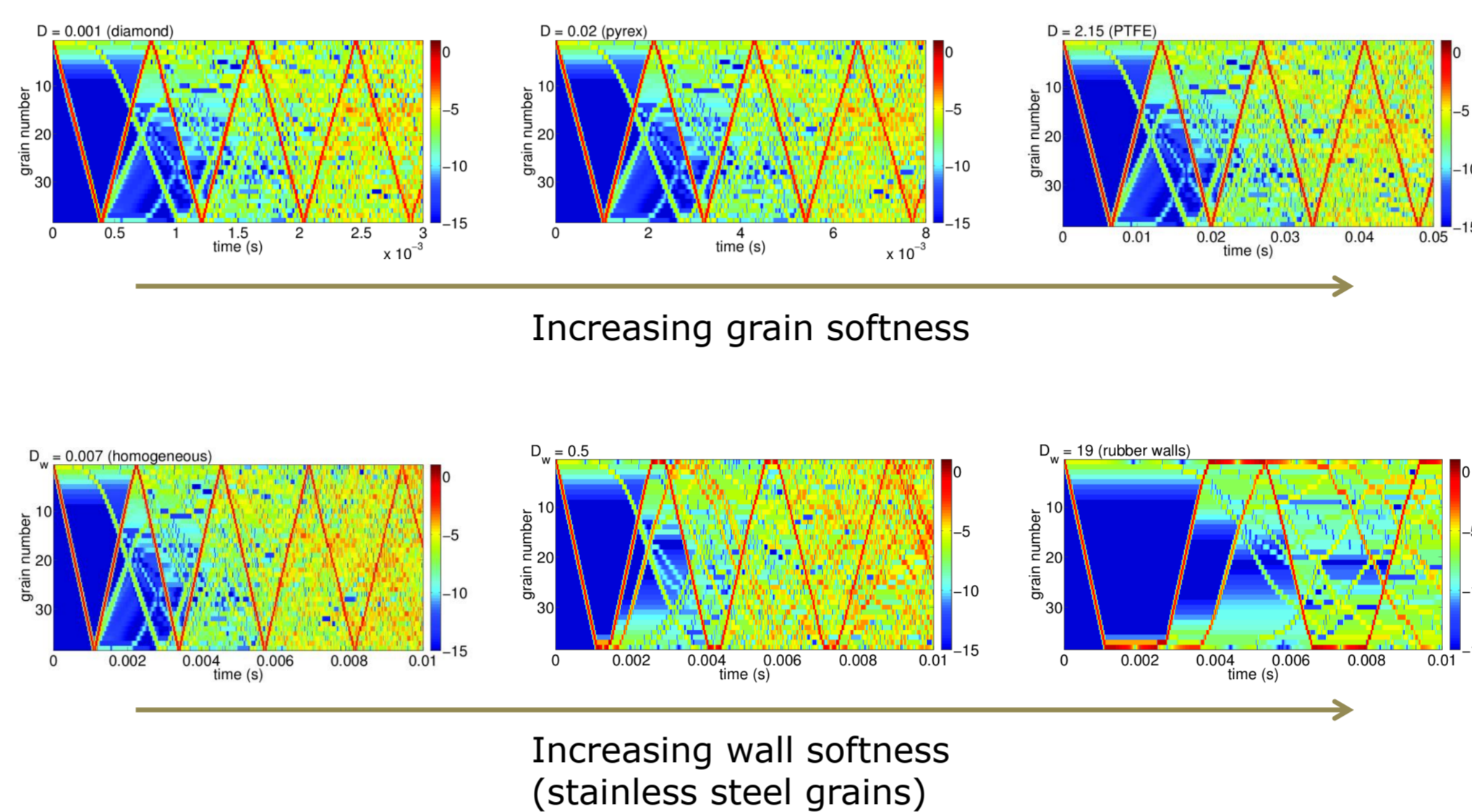


- We then leave the system to evolve in time.
- Equations of motion of the grains are integrated using a standard Velocity-Verlet algorithm.

Results

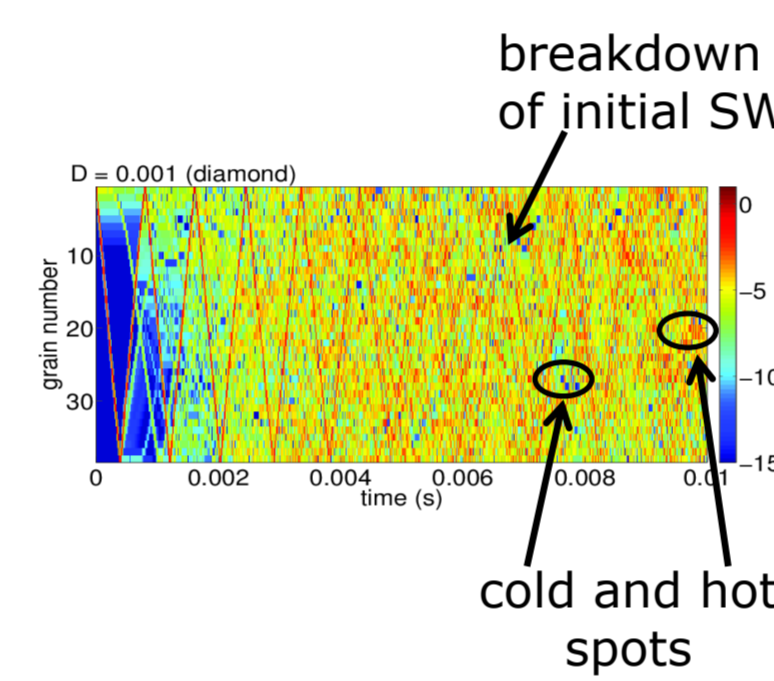
- Short-term behaviour:**

Kinetic energy density plots:



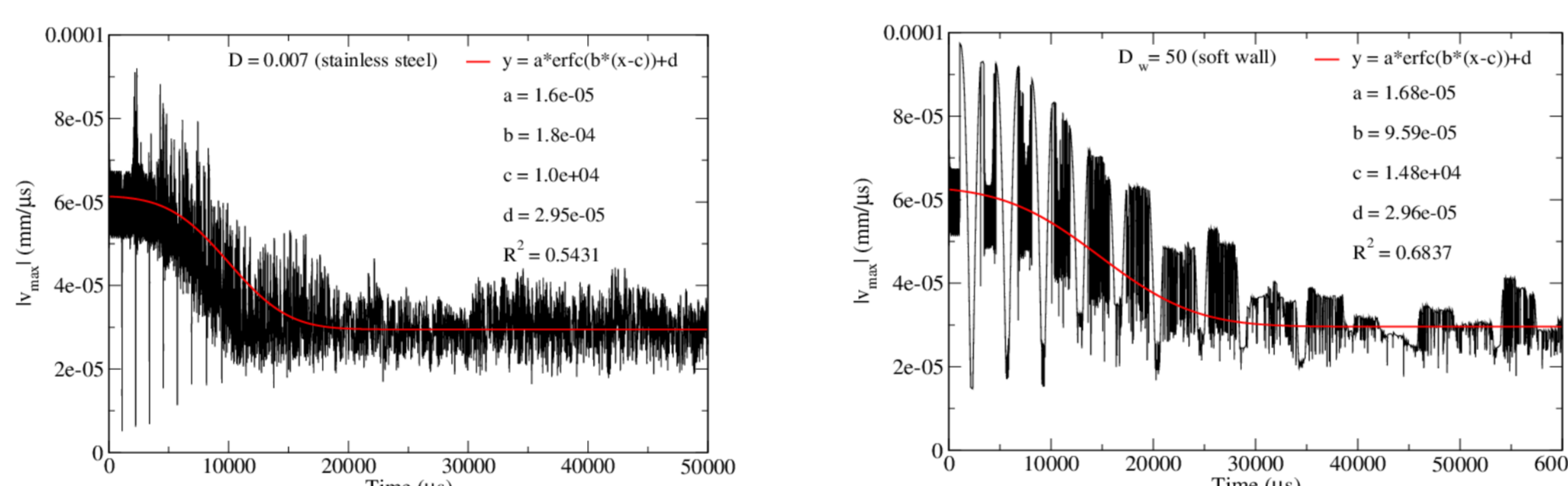
- Transition to quasi-equilibrium:**

Characteristic	Equilibrium	Quasi-equilibrium
Gaussian distribution of velocities	✓	✓
Ergodicity: $\langle K \rangle_N = \langle K \rangle_t$	✓	✓
Dependence on initial conditions	✗	✗
Equipartitioning of energy	✓	✗

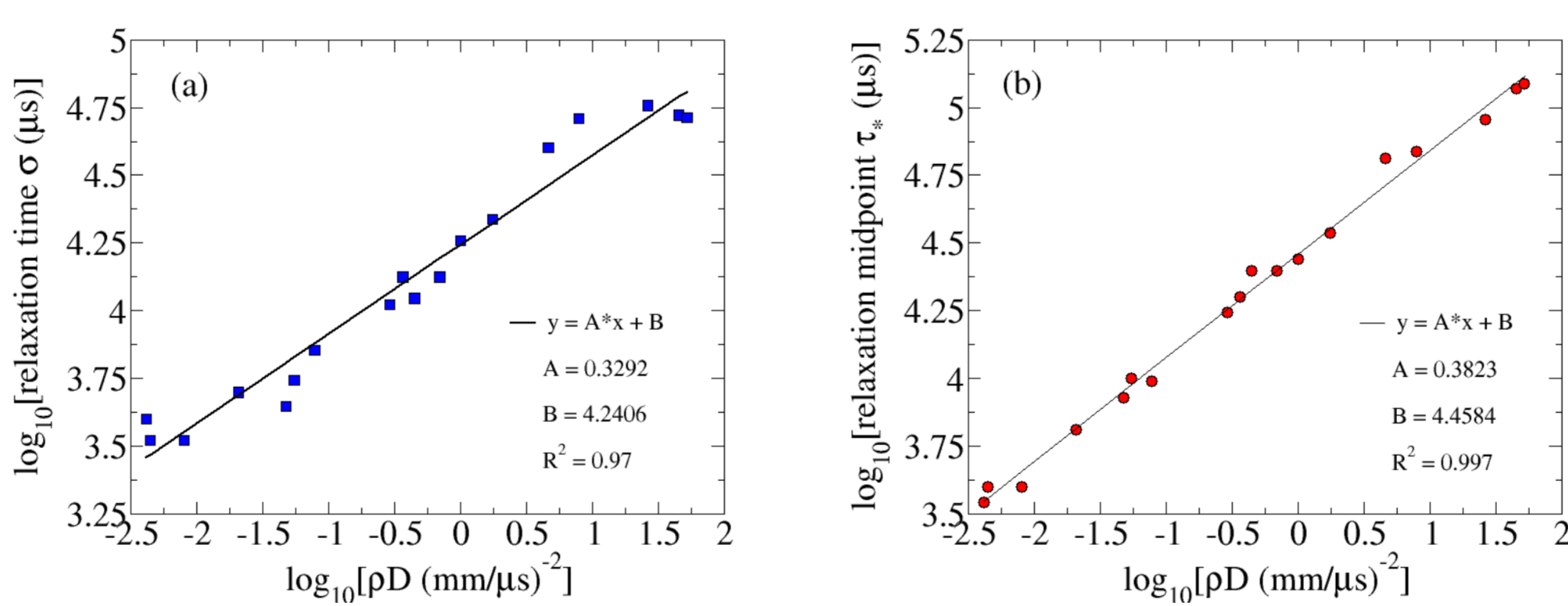


Quantifying the transition:

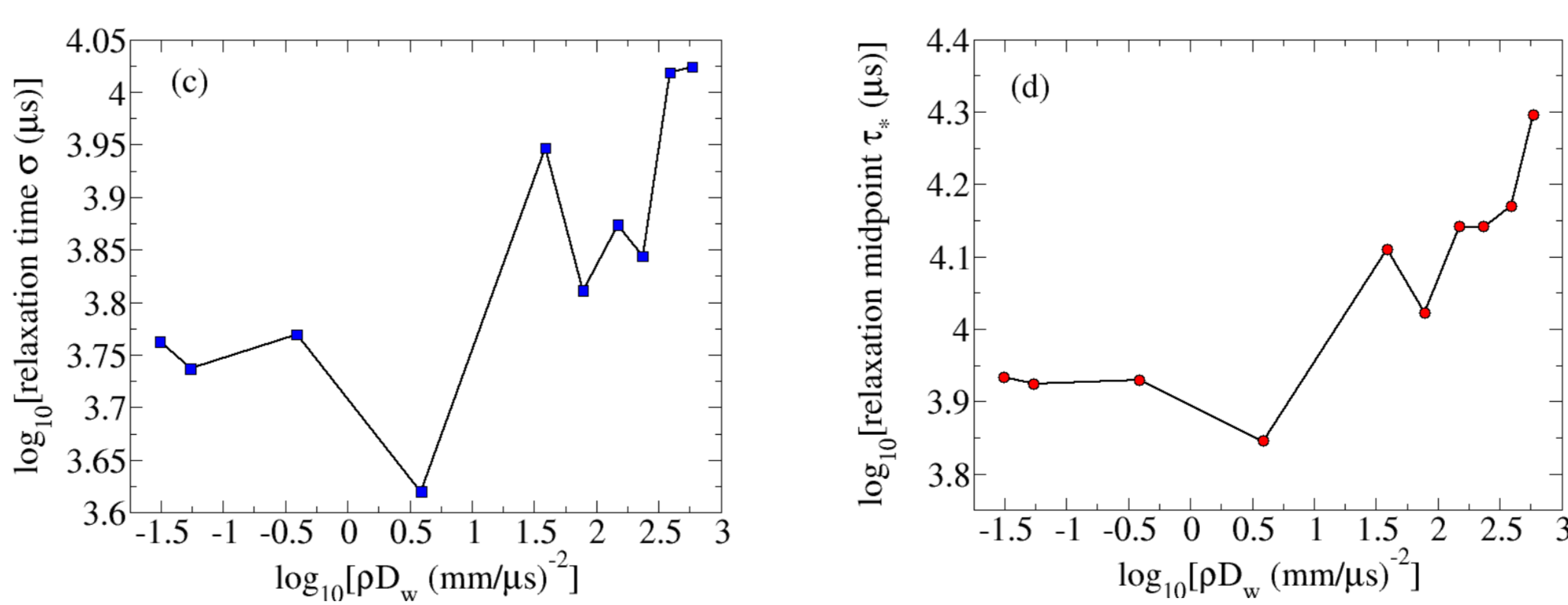
$$|v_{max}| = v_A \left(\operatorname{erfc} \left[\frac{t - \tau_w}{\sigma} \right] \right) + v_B$$



Relaxation rates (homogeneous systems):



Relaxation rates (inhomogeneous systems):



Acknowledgements

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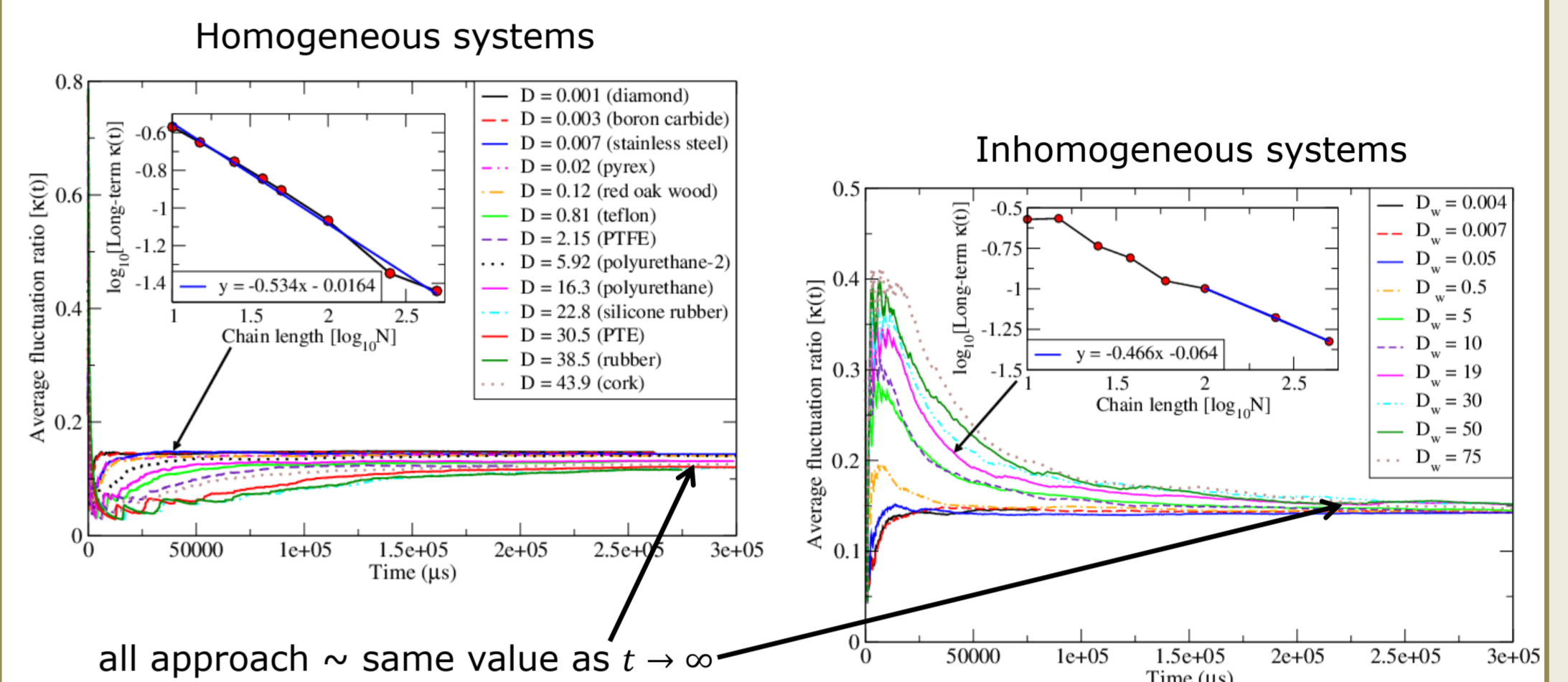
Results cont'd

- Long-term behaviour:**

Kinetic energy fluctuations:

$$\sigma_{KE}(t_m) = \frac{1}{\langle KE \rangle} \sqrt{\frac{1}{t_m} \sum_{t=0}^{t_m} (KE(t) - \langle KE \rangle)^2}$$

$$\kappa(t_M) = (1/M) \sum_{m=1}^M \sigma_{KE}(t_m)$$



Actual equilibrium?

- Extreme long-term behaviour (~ 1-10s):**

Generalized equipartition theorem: $\left\langle \frac{\partial E}{\partial q_i} \right\rangle = \left\langle p_i \frac{\partial E}{\partial p_j} \right\rangle = k_B T \delta_{i,j}$

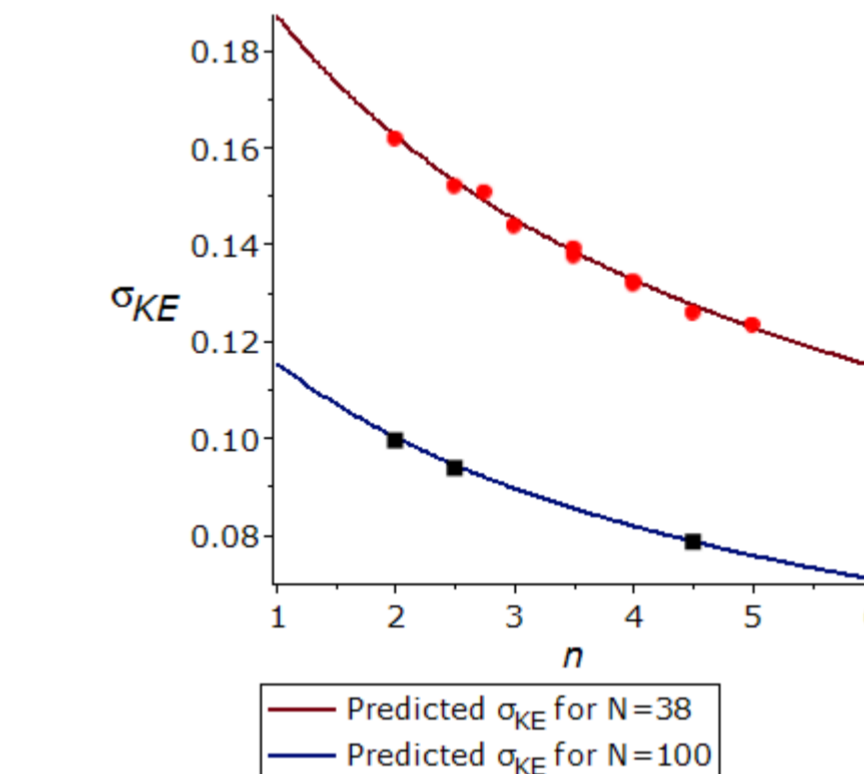
$$E = \frac{1}{2} m v^2 + a \delta^n \rightarrow \langle E_i^v \rangle = \frac{1}{2} k_B T; \langle E_i^{\delta} \rangle = \frac{1}{n} k_B T$$

$$\langle E \rangle = \frac{k_B T}{2} + \frac{k_B T}{n} \rightarrow C_v = \frac{d\langle E \rangle}{dT} = \left(\frac{n+2}{2n} \right) k_B$$

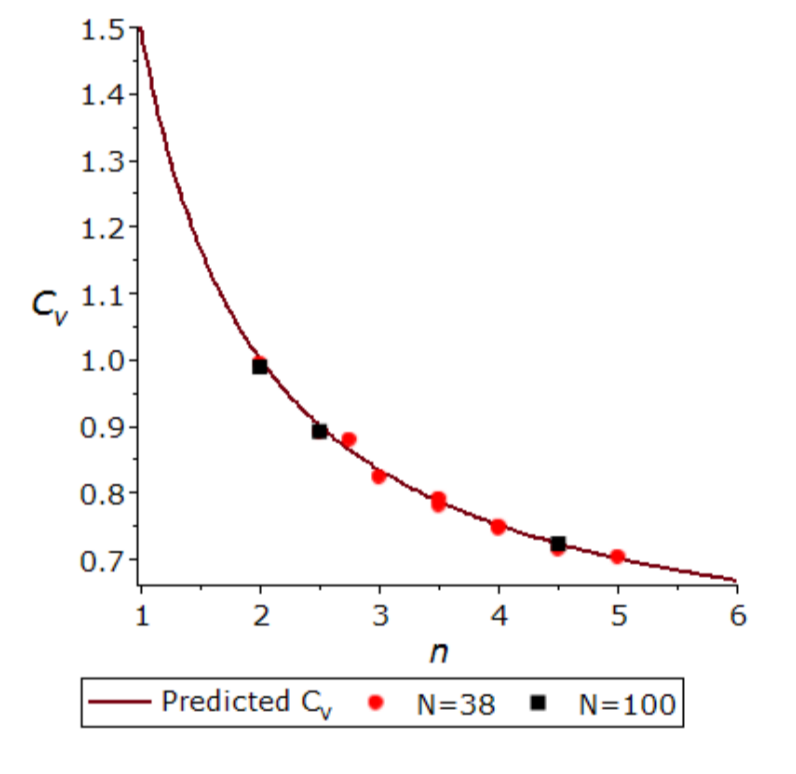
Relating specific heat to kinetic energy fluctuations⁸:

$$\sigma_{KE}^2 = \frac{2}{N} \left(1 - \frac{1}{2C_v} \right) \rightarrow \sigma_{KE} = \sqrt{\frac{2}{N} \left(\frac{2}{n+2} \right)}$$

Kinetic energy fluctuations:



Specific heat:



Conclusions

- Softer grains lead to slower SW propagation speeds.
- Softening the walls introduces a time delay in the reflection of SWs at boundaries, leading to: (1) increased kinetic energy fluctuations in the short term, and (2) a delay in the onset of QEQ, as well as a slowing-down in the rate of relaxation to QEQ.
- Long after the initial energy perturbation, there are an infinite number of SSWs, and the system moves slowly into a true equilibrium state, where energy is equipartitioned among grains and kinetic energy fluctuations can be predicted by generalized equipartition theorem.

References

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