Anomalous Diffusion in Granular Flow: Fractional Kinetics or Intermediate Asymptotics?

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The big picture

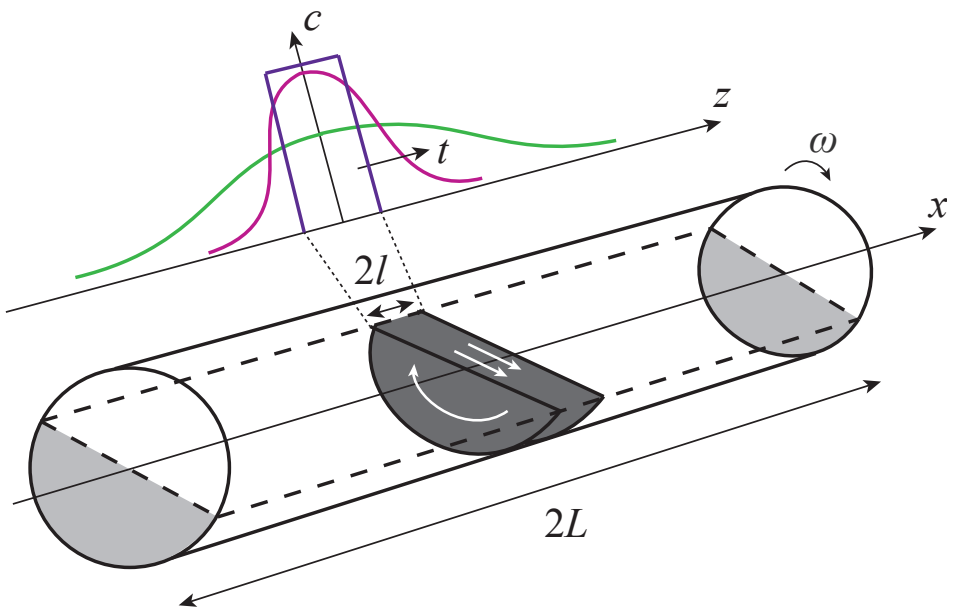
"**Can we develop a general theory of the dynamics of turbulent flows and the motion of granular materials?** *So far, such 'nonequilibrium systems' defy the tool kit of statistical mechanics, and the failure leaves a gaping hole in physics.*" — "So Much More to Know ..." (2005)

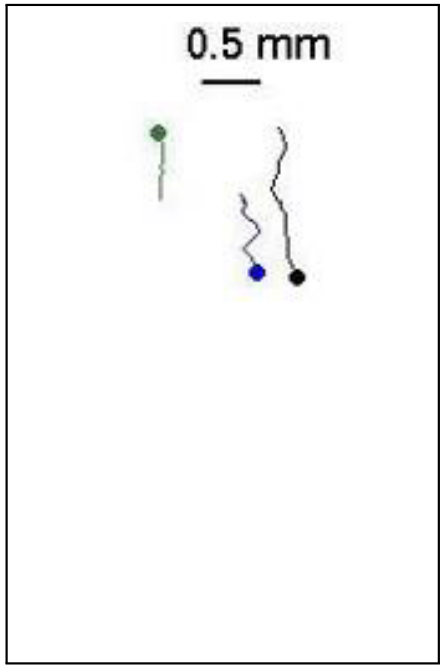
- Motivation:
  - Flowing granular materials — a complex system far from equilibrium.
    - ★ No "general theory" but simple models can be enlightening.
  - Diffusion, rheology, etc. in/of granular flow are not well understood.
- Today:
  1. How/why we observe "diffusion" in granular flows.
  2. Anomalous scalings from "normal" diffusion?

Diffusion of a "granular pulse" in a tumbler

- A band of colored particles in a monodisperse granular mixture diffuses axially as the container is rotated.

  (Lacey, *J. Appl. Chem.* 1954; Carley-Macauly & Donald, *Chem. Eng. Sci.* 1962)
- Many regimes of flow in a tumbler...restrict to continuous flow.
- Thin surface shear layer ⇒ velocity fluctuations ⇒ lateral diffusion.

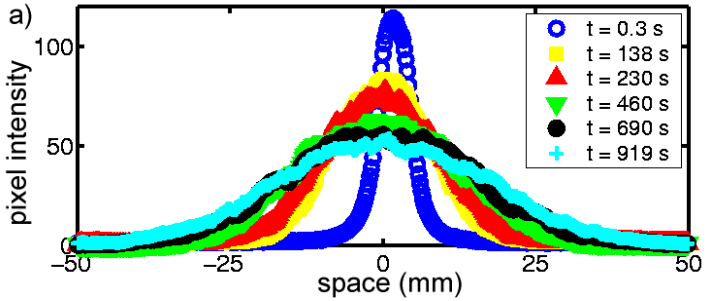


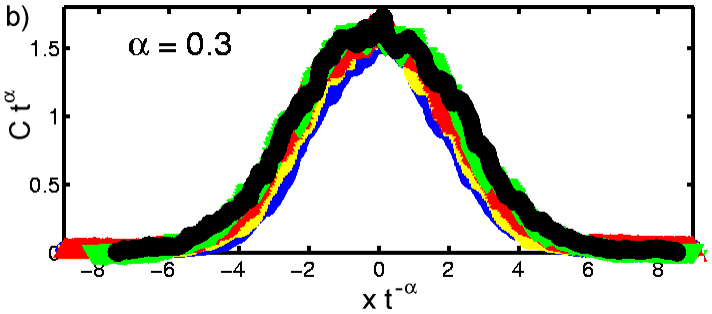


(Khan *et al.*, *New J. Phys.* 2011)

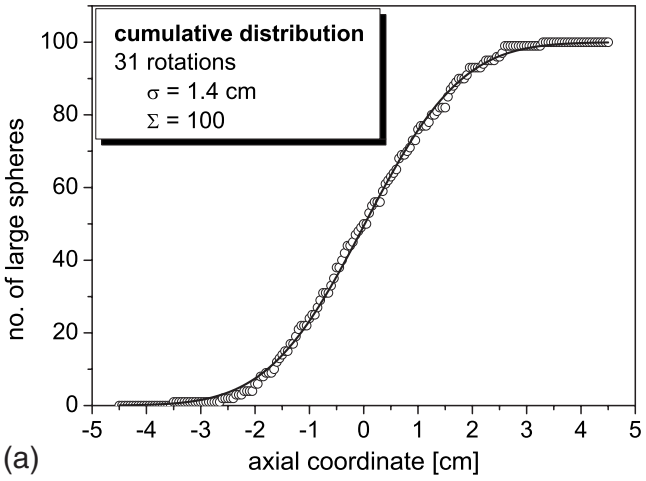
Anomalous macroscopic scalings

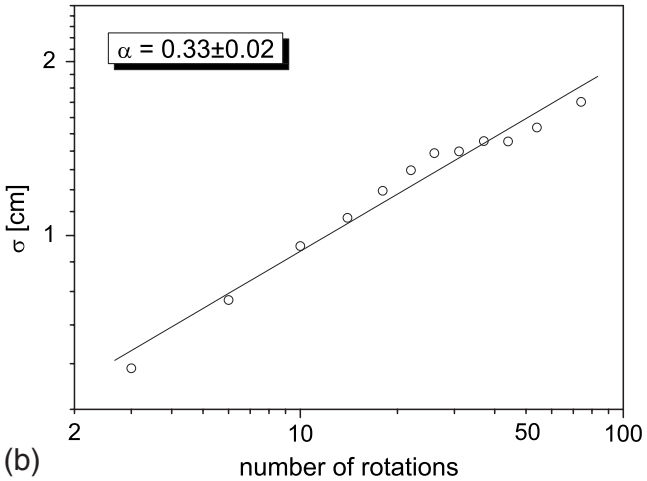
- Experimental concentration profiles of an axially diffusing pulse of dyed black salt grains in white salt grains: (Khan & Morris, *Phys. Rev. Lett.* 2005)





- Experimental concentration profiles of an axially diffusing pulse 4 mm spherical beads in bed of 2mm beads: (Finger *et al.*, *Phys. Rev. E* 2009)





An explanation: Fractional kinetics

- For a random walk with characteristic waiting that diverges, but with finite jump length variance,

$$ {}_0\mathcal{D}_t^{2\alpha} c - \frac{t^{-2\alpha}}{\Gamma(1-2\alpha)} c(x,0) = D_\alpha \frac{\partial^2 c}{\partial x^2}, $$

where $$ {}_0\mathcal{D}_t^{2\alpha} c = \frac{1}{\Gamma(1-2\alpha)} \frac{\partial}{\partial t} \int_0^t \mathrm{d}t' \frac{c(x,t')}{(t-t')^{2\alpha}}, \quad 0 < \alpha < 1/2. $$

- Self-similar solution

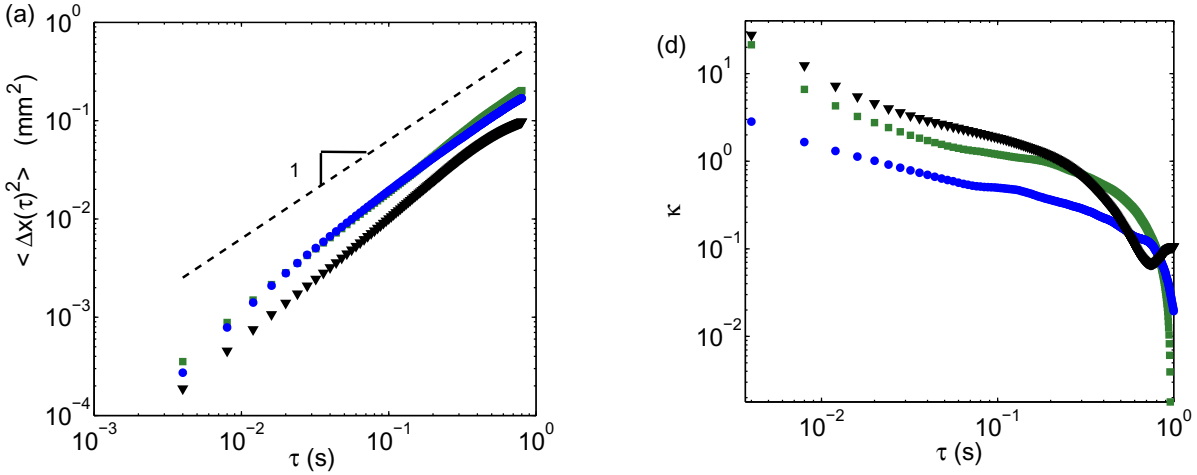
$$ c(x,t) = \frac{1}{\sqrt{4\pi D_\alpha t^{2\alpha}}} F\left(\frac{x}{\sqrt{4 D_\alpha t^{2\alpha}}} \right), \quad F(\xi) = H_{1,2}^{2,0}\left[\xi^2 \middle| \begin{matrix} (1-\alpha, 2\alpha) \\ (0,1), (\frac{1}{2}, 1) \end{matrix} \right], $$

where H is Fox's H-function (Fox, *Trans. Amer. Math. Soc.* 1961).

- $\langle x^2(t) \rangle = \frac{2D_\alpha}{\Gamma(1+2\alpha)} t^{2\alpha}$, $0 < \alpha < 1/2$ ... subdiffusion
$\Rightarrow$ must check in exp't.

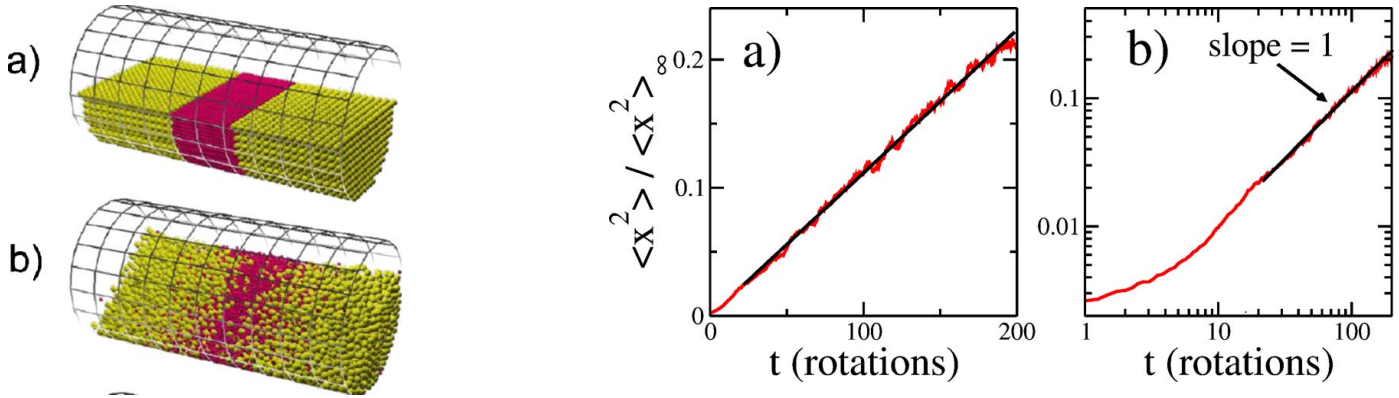
The paradox: Normal microscopic scalings

- Experimental MSD, kurtosis from x-ray imaging (Khan *et al.*, *New J. Phys.* 2011)



- Simulation of 5 mm beads axially diffusing into 10 mm beads:

(Taberlet & Richard, *Phys. Rev. E* 2006)

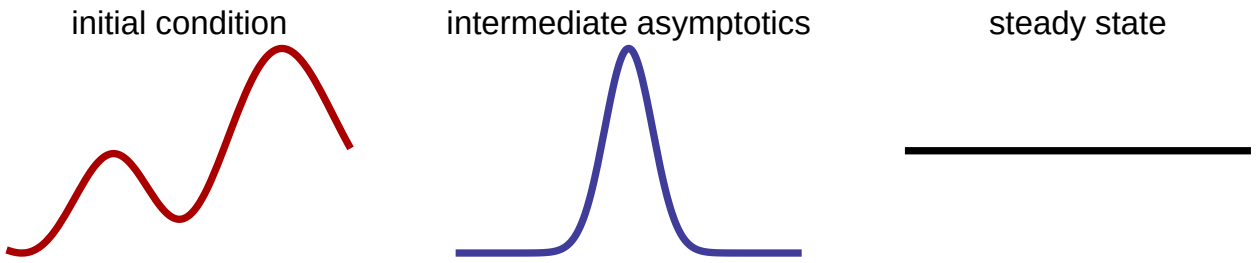


Intermediate asymptotics of diffusion

- Consider dimensionless $[X = x/L,\ T = t/(L^2/D_0)]$ diffusion equation

$$\frac{\partial C}{\partial T} = \frac{\partial}{\partial X}\left(\mathcal{D}\frac{\partial C}{\partial X}\right), \qquad \left.\frac{\partial C}{\partial X}\right|_{X=\pm 1} = 0, \quad C(X,0) = C_i(X).$$

- In general, $\mathcal{D} = \mathcal{D}(C, X, \cdots)$.
- $\mathcal{D} = 1$: random walk with $\langle(\Delta X)^2\rangle \propto t$. (Einstein, *Ann. Phys.* 1905)
  - C-dependent jump probability leads to $\mathcal{D}(C)$. (Boon & Lutsko, *EPL* 2007)
- Similarity solution of the form $C(X,T) = T^{-1/2}\mathfrak{C}(XT^{-1/2})$.



(Barenblatt, *Scaling, Self-similarity, and Intermediate Asymptotics*, 1996)

Optimal self-similar solution (I)

- Let $\tau = T + T^*$ and $\eta = (X + X^*)/\sqrt{4(T + T^*)}$, then diffusion eq. becomes
$$\tau \frac{\partial C}{\partial \tau} = \frac{\eta}{2}\frac{\partial C}{\partial \eta} + \frac{1}{4}\frac{\partial^2 C}{\partial \eta^2}.$$
- Separate variables as $C(\tau, \eta) = \tau^{-\lambda} g_\lambda(\eta)$ to get
$$g_\lambda'' + 2\eta g_\lambda' + 4\lambda g_\lambda = 0 \quad \Rightarrow \quad g_\lambda(\eta) = \mathrm{e}^{-\eta^2} \underbrace{\mathcal{H}_n(\eta)}_{\text{Hermite}}, \quad \lambda = \frac{n+1}{2}.$$
- For some A_n determined from the I.C., the general solution is
$$C(\eta, T) = \mathrm{e}^{-\eta^2} \sum_{n=0}^{\infty} \frac{A_n}{(T + T^*)^{\frac{n+1}{2}}} \mathcal{H}_n(\eta).$$

(Zel'dovich & Barenblatt, *Dokl. Akad. Nauk. SSSR* 1958;

Kleinstein & Ting, *ZAMM* 1971; Witelski & Bernoff, *Stud. Appl. Math.* 1998)

- But...I didn't tell you what T^* and Z^* are!

Optimal self-similar solution (II)

- Pick T^* and X^* so that $A_1 = A_2 = 0$, then solutions for arbitrary initial data can be well-approximated (for $\mathcal{D} = 1$ and $T > T^*$) by the point-source similarity solution

$$C(X,T) = \frac{1}{\sqrt{4\pi(T+T^*)}} \exp\left\{-\frac{(X+X^*)^2}{4(T+T^*)}\right\} + \mathcal{O}\left(\frac{1}{T^2}\right)$$

provided that

$$X^* = -\frac{M_1}{M_0}, \quad T^* = \frac{1}{2}\left[\frac{M_2}{M_0} - \left(\frac{M_1}{M_0}\right)^2\right],$$

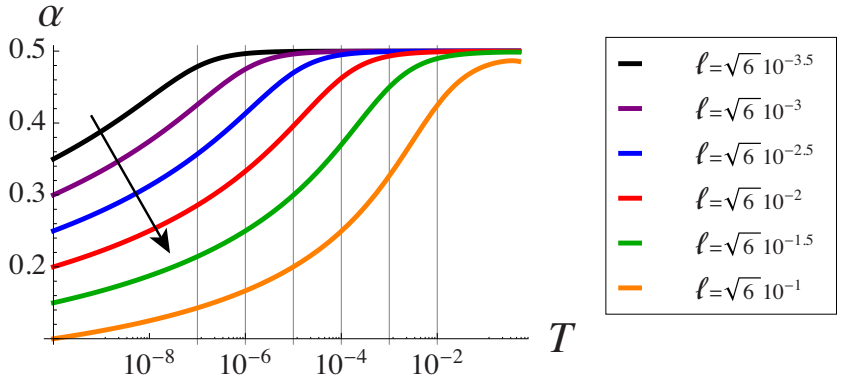
and $M_k := \int_{-\infty}^{+\infty} C_i(X)\, X^k \,\mathrm{d}X$.

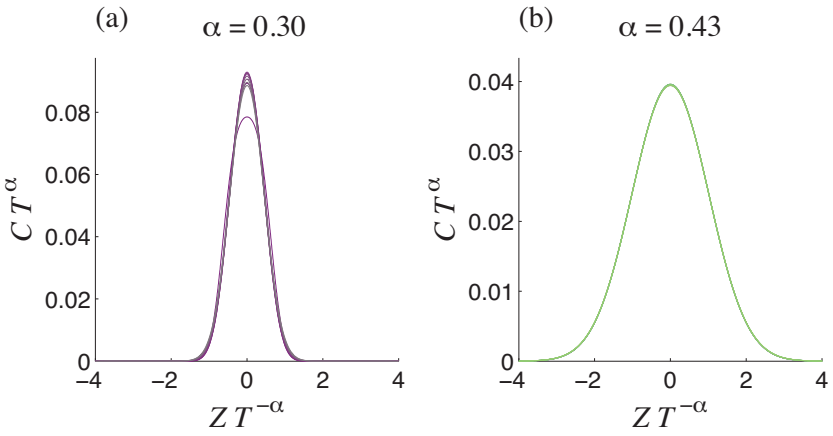
- Note: $Z^* = 0$ in this talk (symmetric initial conditions only).

Time-dependent anomalous collapse exponents

- Data collapses under rescaling $C(X,T) \to C(X/T^{\alpha},T)T^{\alpha}$.
- $\Rightarrow$ we are balancing T^{α} with $\sqrt{T+T^*}$, meaning

$$\alpha(T) \simeq \frac{\ln(T+T^*)}{2\ln T} = \begin{cases} \frac{1}{\ln T}\left[\ln T^* + \frac{T}{2T^*} + \mathcal{O}(T^2)\right], & T \to 0, \\ \frac{1}{2} + \frac{1}{\ln T}\left[\frac{T^*}{2T} + \mathcal{O}(T^{-2})\right], & T \to \infty. \end{cases}$$





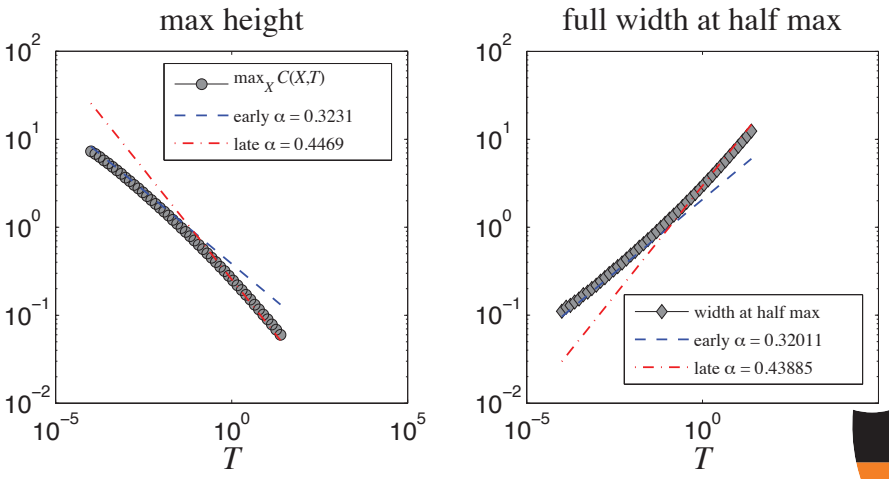
(Christov & Stone, *Proc. Natl Acad. Sci. USA* 2012)

Concentration-dependent diffusivity in bidisperse mixtures

- Suppose C is the concentration of larger particles, then $\mathcal{D}(C) = 1 + (C - 1/2)$. (Ristow & Nakagawa, *Phys. Rev. E* 1999)
- Seeking a self-similar solution $C(X,T) = T^{-\alpha}\mathfrak{C}(\zeta)$ with $\zeta = T^{-\alpha}X$:

$$0 = \mathfrak{C} + \zeta\mathfrak{C}' + \underbrace{\frac{1}{2\alpha}T^{1-2\alpha}\mathfrak{C}''}_{①} + \underbrace{\frac{1}{2\alpha}T^{1-3\alpha}\left(\mathfrak{C}^2\right)''}_{②}.$$

- If $\alpha = 1/3$, then $T^{1-2\alpha} = T^{1/3} \ll 1$ for $T \ll 1$.
- If $\alpha = 1/2$, then $T^{1-3\alpha} = T^{-1/2} \ll 1$ for $T \gg 1$.



- Q: Find $\alpha(T)$ in the crossover regime? [Christov, Eggers, Stone (in prep)]

Summary

- What we have done:
  - Everyone can be right! (Proposed a resolution to the granular diffusion "paradox.")
  - Analytical foundations for anomalous exponents in Fickian diffusion.
- What we haven't done:
  - Find an asymptotic solution matching across both scaling regimes in the nonlinear case?
  - Take into account the disparate flow regimes (thin shear layer on top of bulk in solid body rotation)?

Thank you for your attention!


PNAS

Resolving a paradox of anomalous scalings in the diffusion of granular materials

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