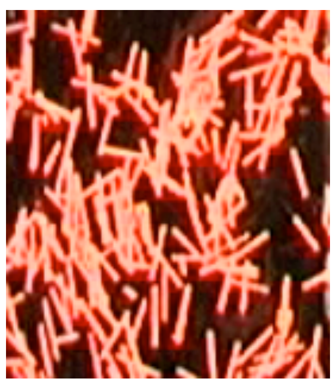
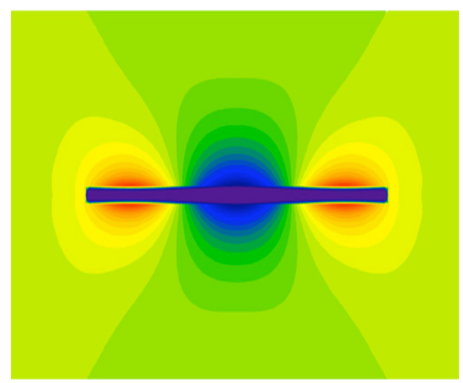
Collective dynamics in dispersions of anisotropic and deformable particles

David Saintillan

Courant Institute of Mathematical Sciences, New York University

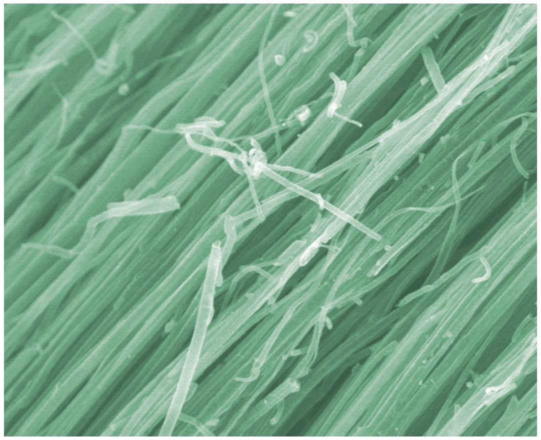
Thesis advisors: Eric Shaqfeh & Eric Darve (Stanford University)





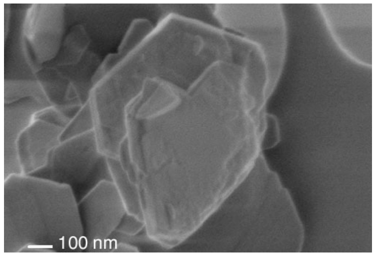
Acrivos Award Lecture, APS/DFD, Salt Lake City 2007

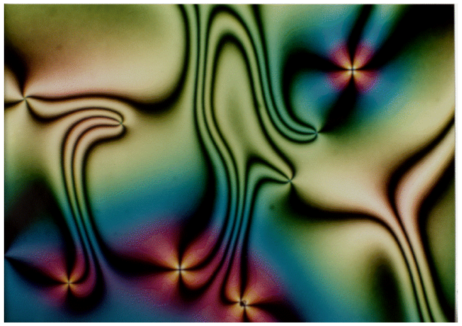
Outline



- **The sedimentation of orientable particles**
  - *The instability of sedimenting fibers*
  - *Point particle simulations*
  - *Mechanism for wavenumber selection*
  - *Case of deformable particles*

- **Induced-charge electrophoresis of polarizable rods**
  - *Motivation: micro-barcode analysis*
  - *Physics and theoretical model*
  - *Brownian dynamics simulations*

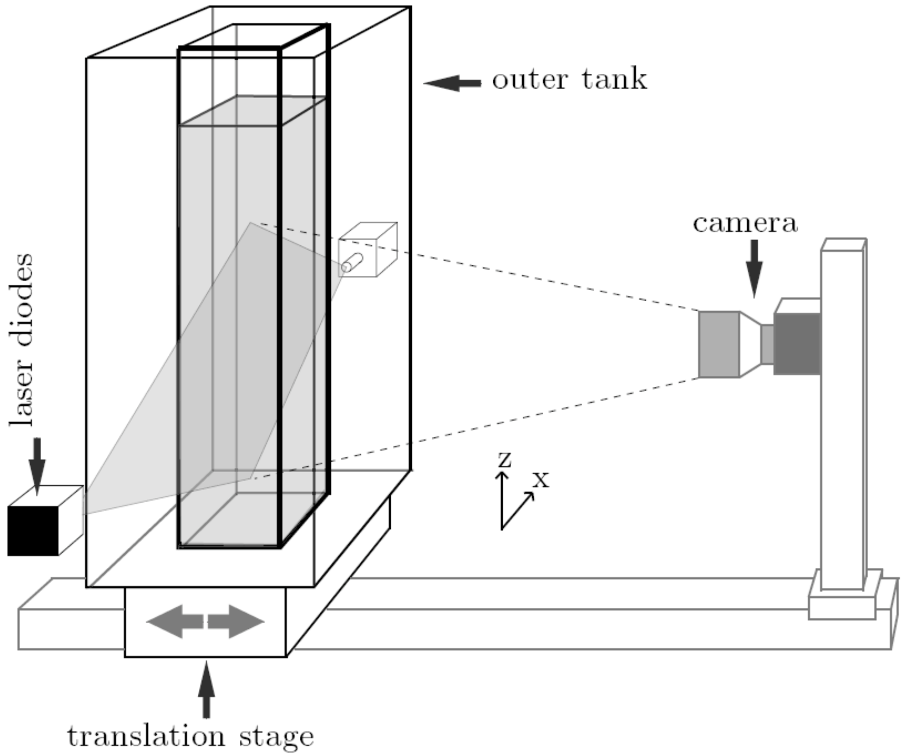




Fluctuations in suspensions of fibers

Experiments by Guazzelli and coworkers:

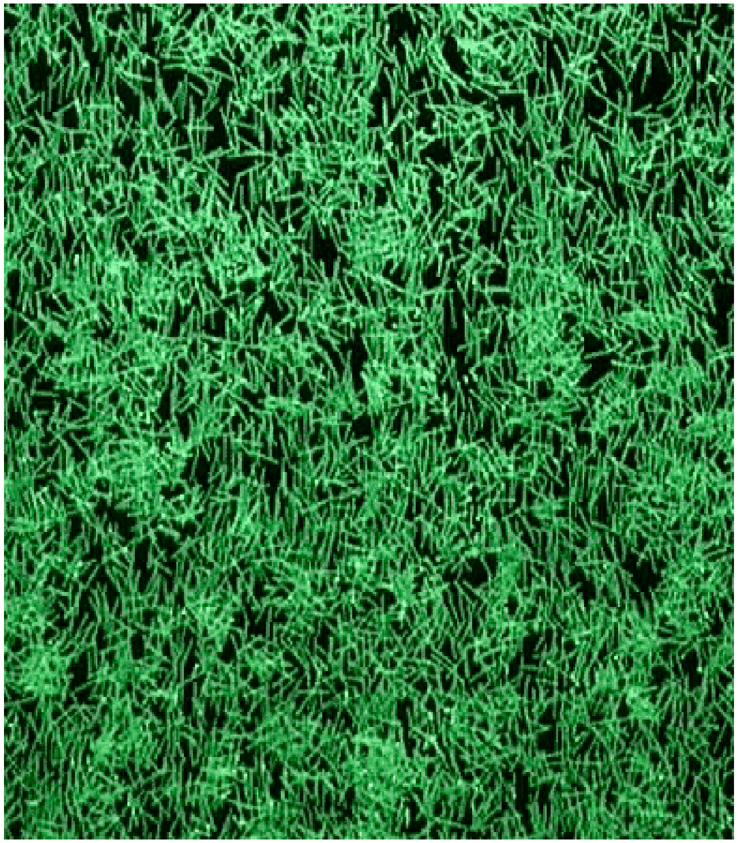
- **Fibers aggregate into dense clusters or streamers, separated by clarified regions.**
- **Strong impact on sedimentation statistics: enhanced sedimentation rate and velocity fluctuations in dilute regime.**



Nylon fibers in silicon oil

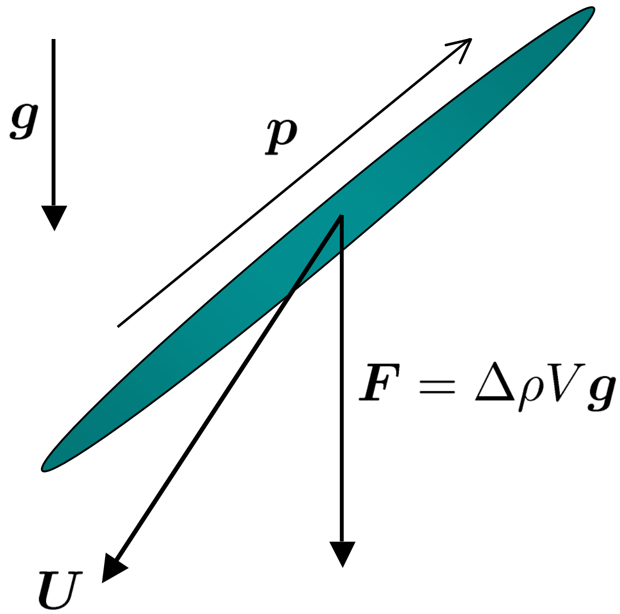
Aspect ratio : $A = 15$

Volume fraction : $\phi = 0.5\,\%$



Herzhaft, Guazzelli, Mackaplow & Shaqfeh, *PRL* (1996)
Herzhaft & Guazzelli, *JFM* (1999)
Metzger, Guazzelli & Butler, *PRL* (2005)
Metzger, Butler & Guazzelli, *JFM* (2006)

Instability mechanism



- **Sedimentation velocity:**

$$\boldsymbol{U} = \boxed{\mathbf{M}} \cdot \boldsymbol{F}$$

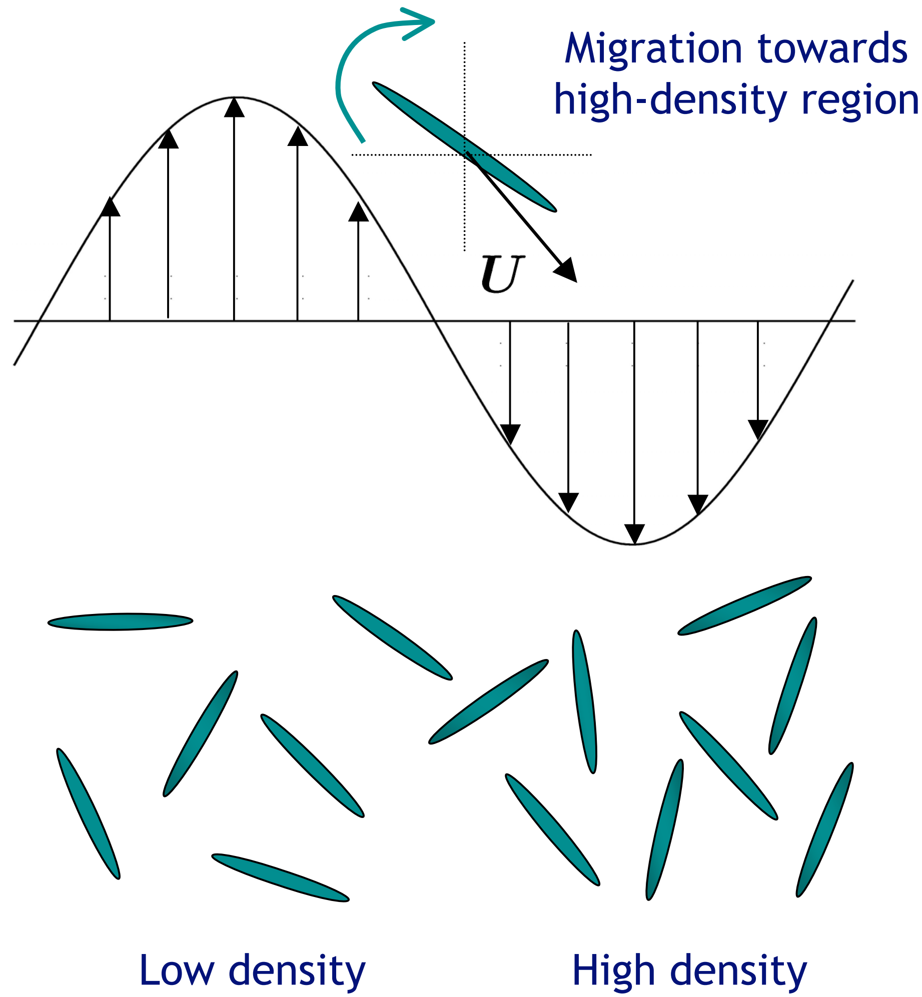
mobility tensor

- **For an axisymmetric particle:**

$$\mathbf{M} = \beta_0 \mathbf{I} + \beta_1 \boldsymbol{pp}$$

⇨ **lateral motion typically occurs**

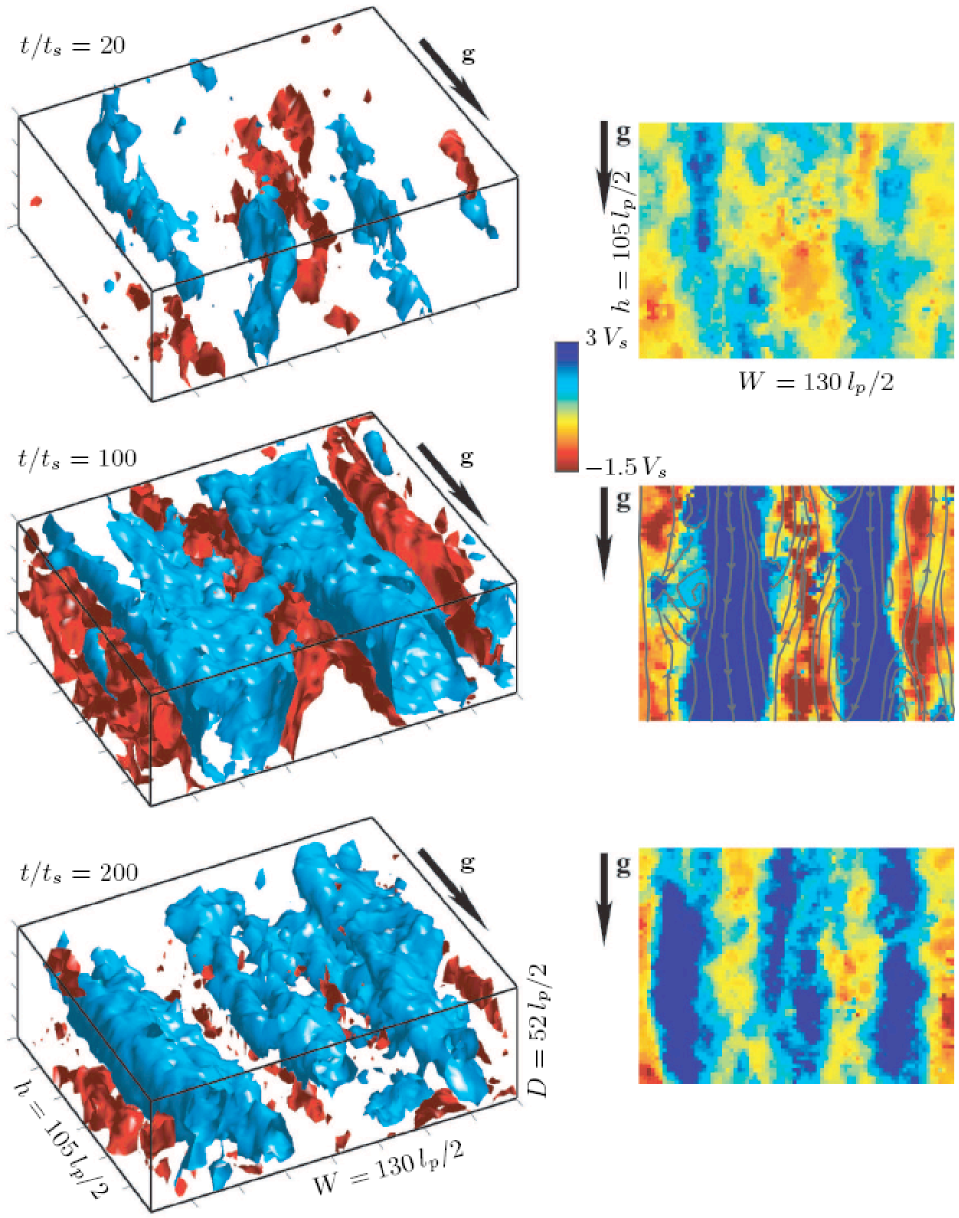
Koch & Shaqfeh, *J. Fluid Mech.* 1989



Wavenumber selection in experiments

Experiments show a transition from one large streamer toward mutliple streamers in the lateral direction, not captured by previous theoretical and numerical studies.

What is the mechanism for this wavenumber selection?

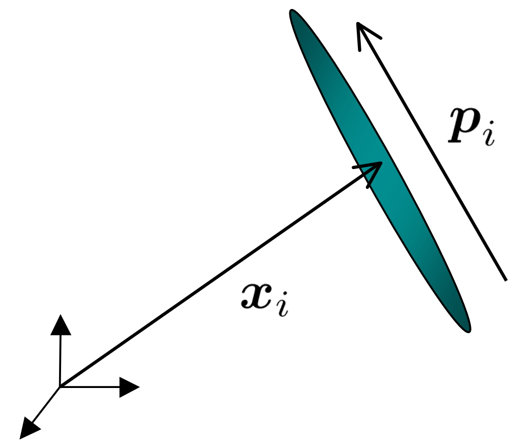


Metzger, Guazzelli & Butler, *PRL* (2005)
Metzger, Butler & Guazzelli, *JFM* **575** 307 (2007)

Point particle simulations: method

- **Dynamic equations** for the particle motions

$$\begin{cases} \dot{\boldsymbol{x}}_i = (\beta_0 \mathbf{I} + \beta_1 \boldsymbol{p}_i \boldsymbol{p}_i) \cdot \boldsymbol{F} + \boldsymbol{u}(\boldsymbol{x}_i) \\ \dot{\boldsymbol{p}}_i = (\mathbf{I} - \boldsymbol{p}_i \boldsymbol{p}_i) \cdot \left(\dfrac{A^2 - 1}{A^2 + 1} \mathbf{E} + \boldsymbol{\Omega} \right) \cdot \boldsymbol{p}_i \end{cases}$$



- **Disturbance velocity**

$$-\mu \nabla^2 \boldsymbol{u} + \boldsymbol{\nabla} p = \boldsymbol{f}, \quad \boldsymbol{\nabla} \cdot \boldsymbol{u} = \boldsymbol{0}$$

$$\boldsymbol{f}(\boldsymbol{x}) = \sum_{i=1}^{N} \boldsymbol{F} M(x - x_i) M(y - y_i) M(z - z_i)$$

(B-spline interpolation)

- **Solution of the Stokes equation**

Sum of Fourier modes satisfying no normal velocity BC on walls (slip is allowed)

(Bergougnoux et al., *Phys. Fluids* 2003)

$$\begin{cases} \boldsymbol{u}(\boldsymbol{x}) = \displaystyle\sum_{i,j,k} \hat{u}_{ijk} \times \begin{Bmatrix} \dfrac{ik}{d_x d_z} \sin\left(\dfrac{\pi i x}{d_x}\right) \cos\left(\dfrac{\pi j y}{d_y}\right) \cos\left(\dfrac{\pi k z}{d_z}\right) \\ \dfrac{jk}{d_y} \cos\left(\dfrac{\pi i x}{d_x}\right) \sin\left(\dfrac{\pi j y}{d_y}\right) \cos\left(\dfrac{\pi k z}{d_z}\right) \\ -\left(\dfrac{i^2}{d_x^2} + \dfrac{j^2}{d_y^2}\right) \cos\left(\dfrac{\pi i x}{d_x}\right) \cos\left(\dfrac{\pi j y}{d_y}\right) \sin\left(\dfrac{\pi k z}{d_z}\right) \end{Bmatrix} \\ \hat{u}_{ijk} = \dfrac{\hat{f}_{ijk}}{\pi^2 \left[\left(\frac{i}{d_x}\right)^2 + \left(\frac{j}{d_y}\right)^2 + \left(\frac{k}{d_z}\right)^2 \right]^2} \end{cases}$$

Saintillan, Shaqfeh & Darve, *J. Fluid Mech.* **553**, 347 (2006)

Point particle simulations in bounded containers

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Aspect ratio

$A = 15$

Volume fraction

$\phi = 0.5\,\%$

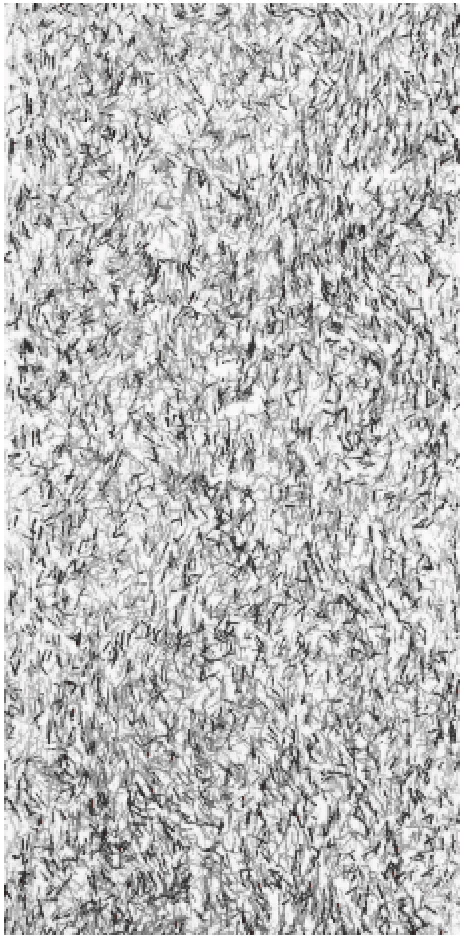
Box dimensions

$32 \times 12 \times 180$

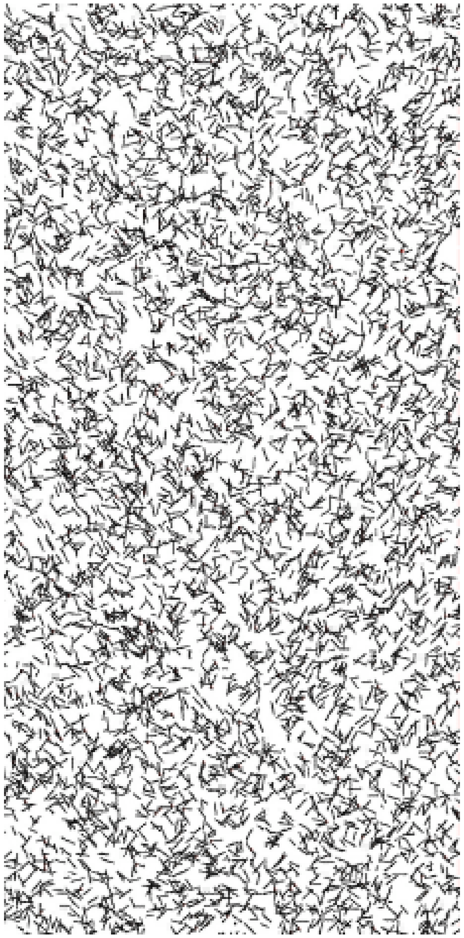
$\sim 150,000$ particles

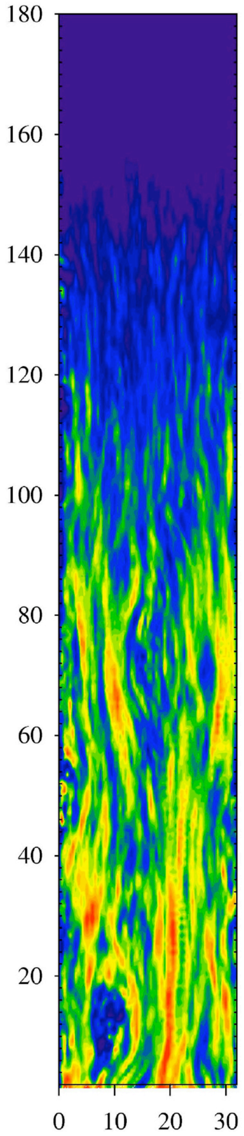
Experiment: movie courtesy of Bloen Metzger, Elisabeth Guazzelli (IUSTI, CNRS), and Jason Butler (U. Florida)

Experiment



Simulation

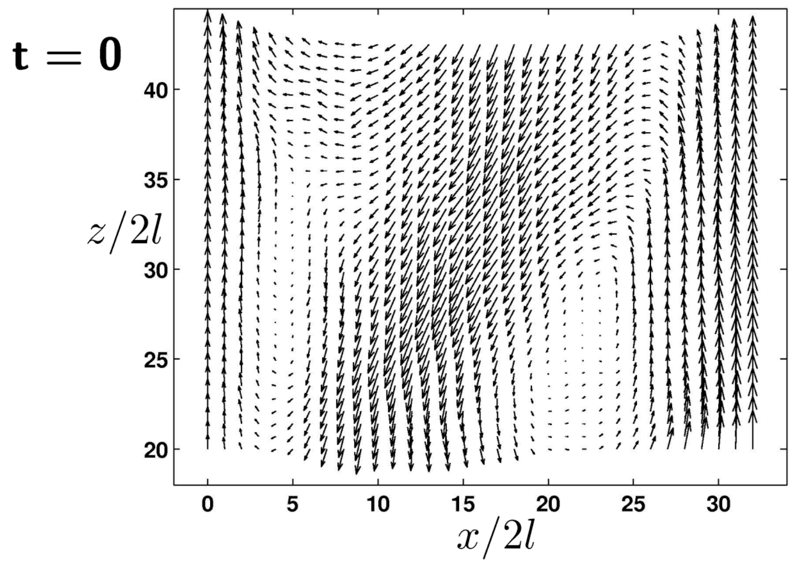


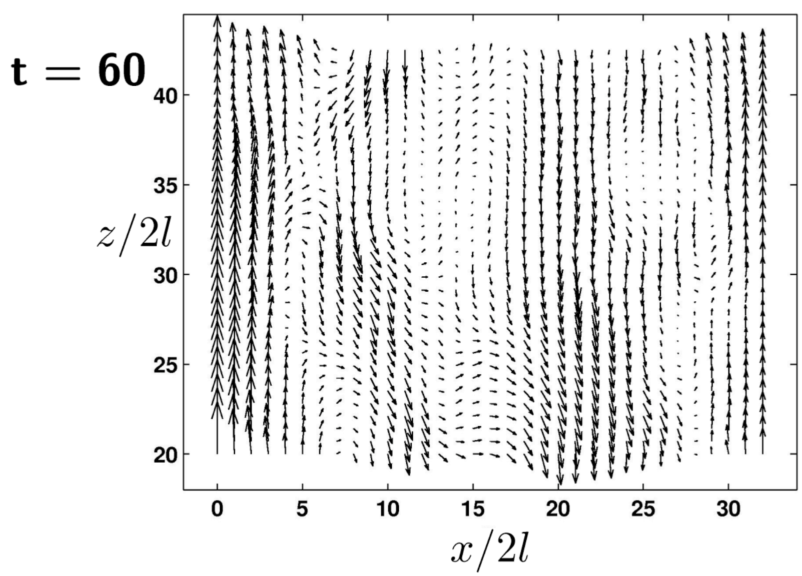


Disturbance velocity autocorrelation function

$A = 15 \quad \phi = 0.2\ \%$

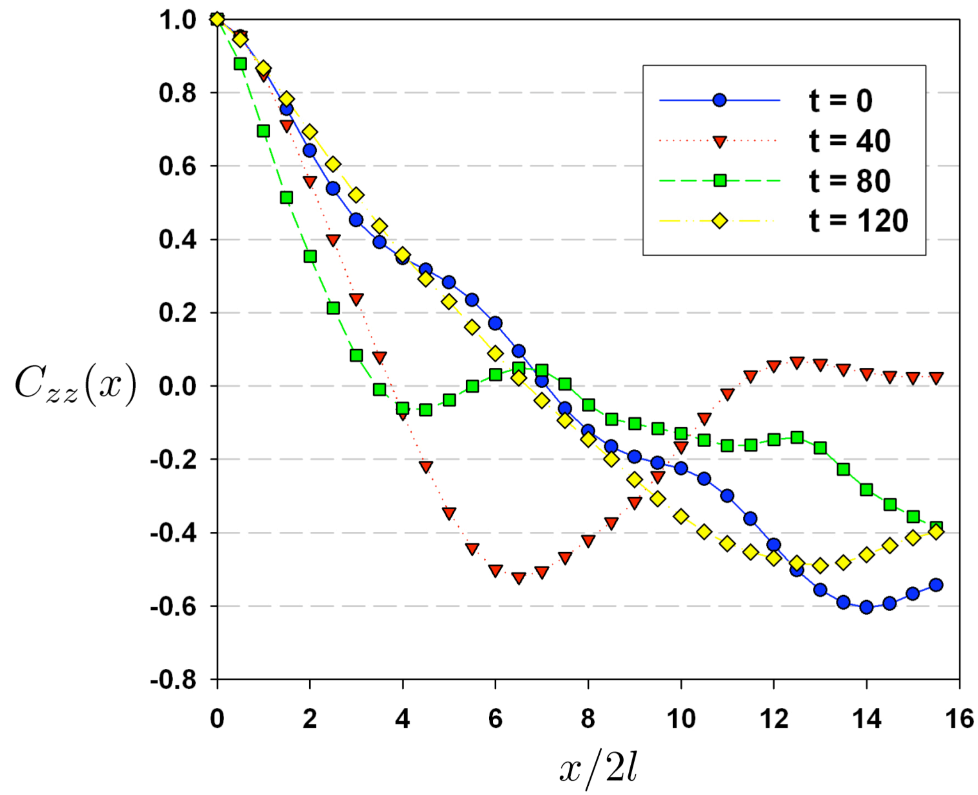
box : $32 \times 12 \times 180 \quad 59,904$ particles





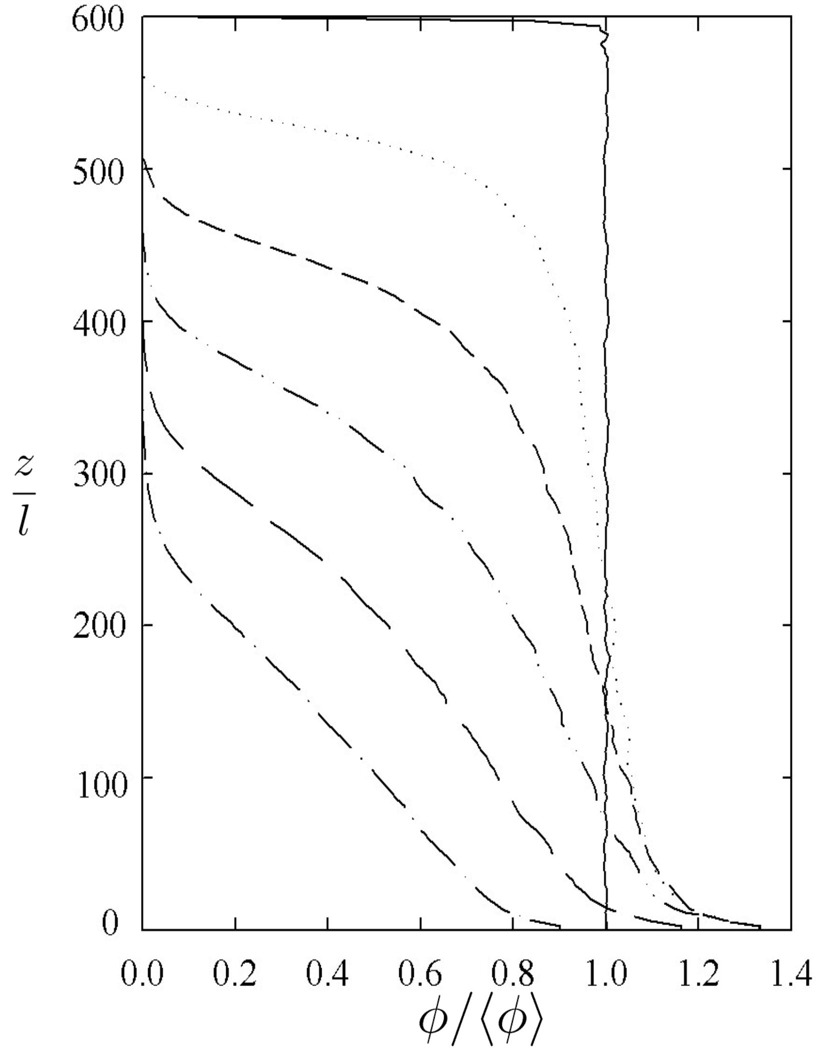
Autocorrelation function in the horizontal direction of the vertical component of the velocity field

$$C_{zz}(x) = \int u_z(x')u_z(x'+x)\mathrm{d}x'$$



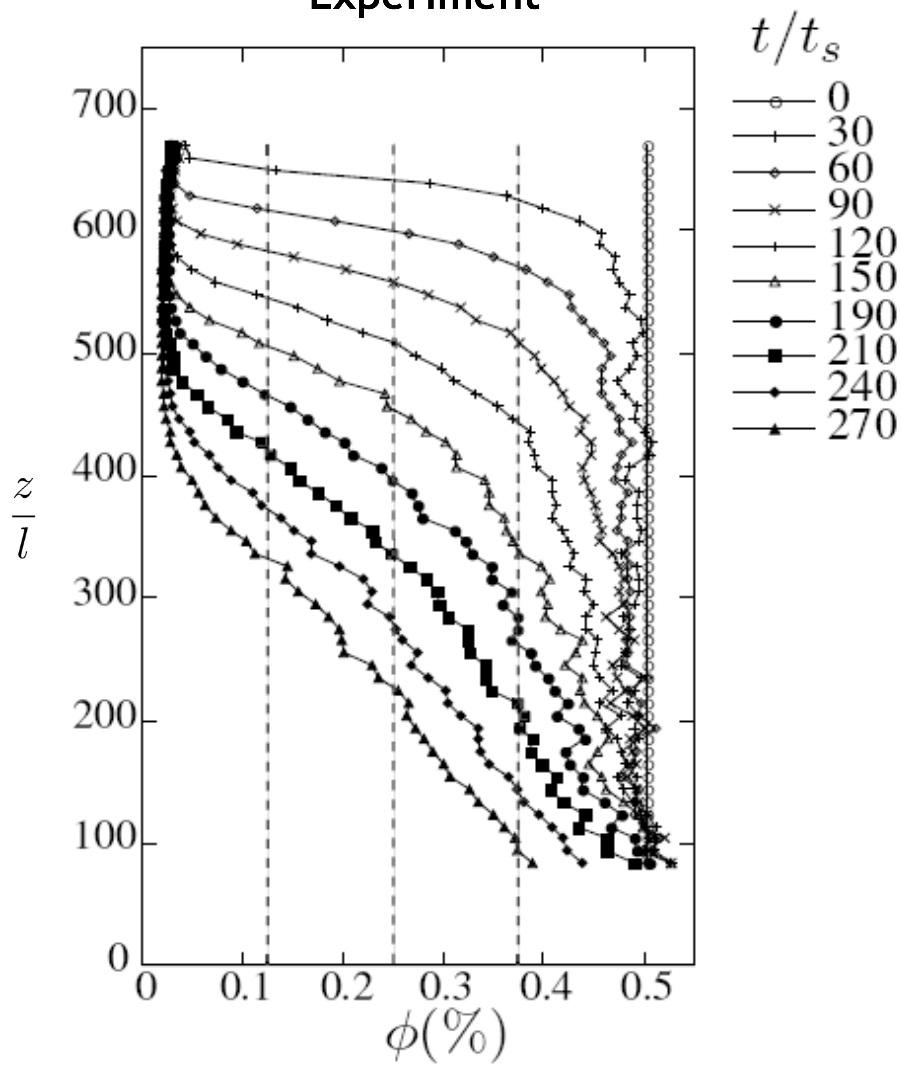
Stratification

Simulation



Saintillan, Shaqfeh, Darve, *Phys. Fluids* **18** 121503 (2006)

Experiment

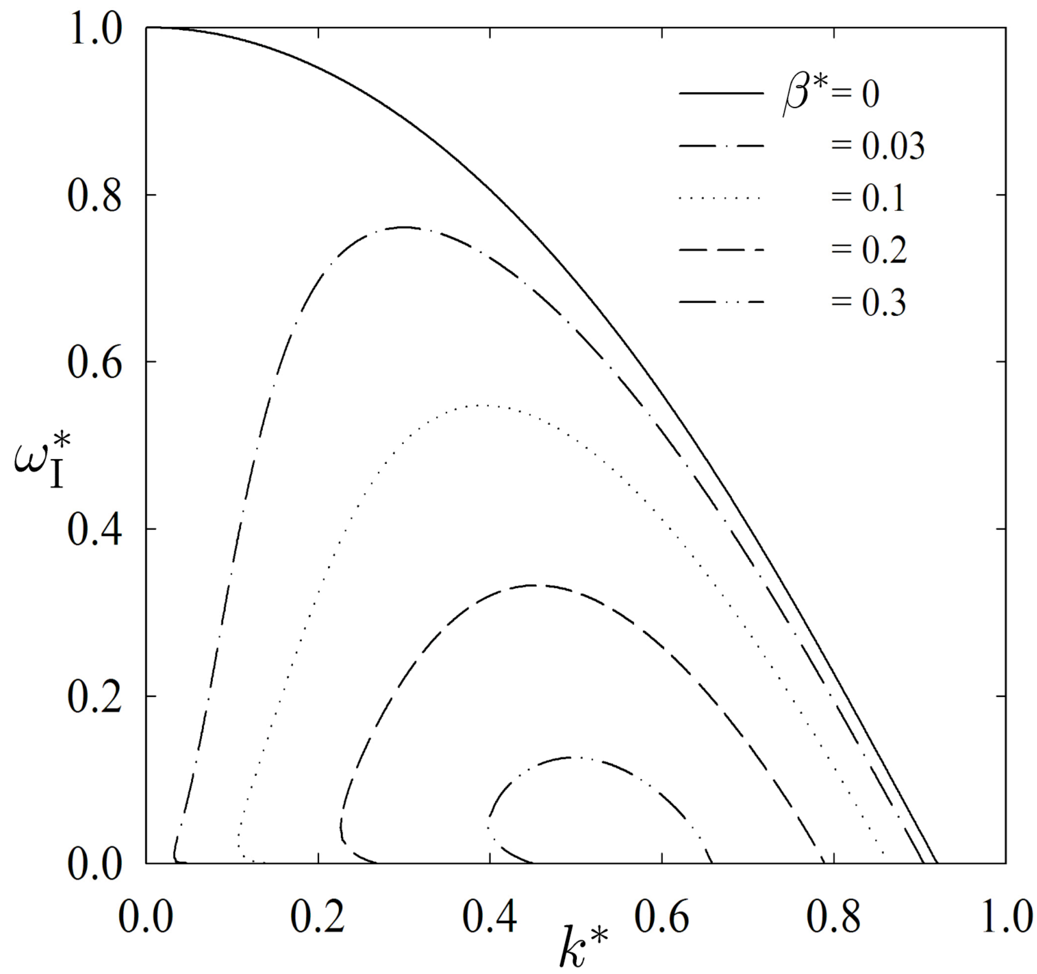


Metzger, Butler & Guazzelli, *JFM* **575** 307 (2007)

Effect of stratification: Linear stability analysis

Consider fluctuations with respect to a linearly stratified background concentration:

$$\begin{cases} c(\boldsymbol{x},\boldsymbol{p},0) = \dfrac{n}{4\pi}(1-\beta z) + \epsilon\tilde{c}(\boldsymbol{k},\boldsymbol{p},t)\mathrm{e}^{\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{x}-\omega t)} \\ (\beta > 0,\ \beta^{-1} \gg L) \end{cases}$$



Analysis of the dispersion relation yields the following scaling for the most unstable wavenumber:

$$\boxed{kl \sim \phi^{1/5}(\beta l)^{2/5}}$$

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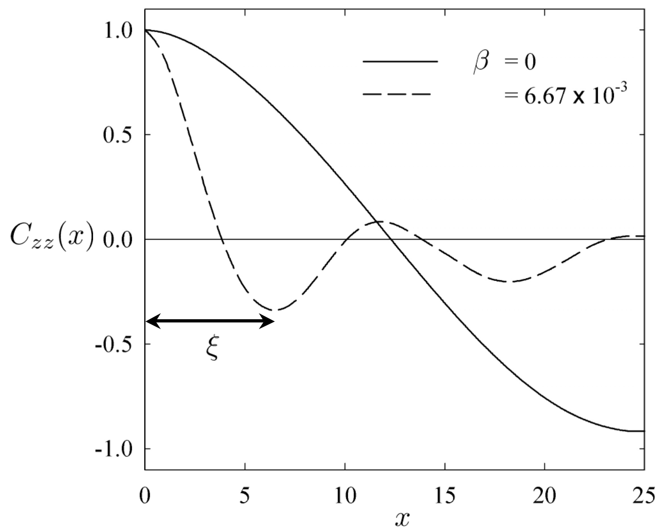
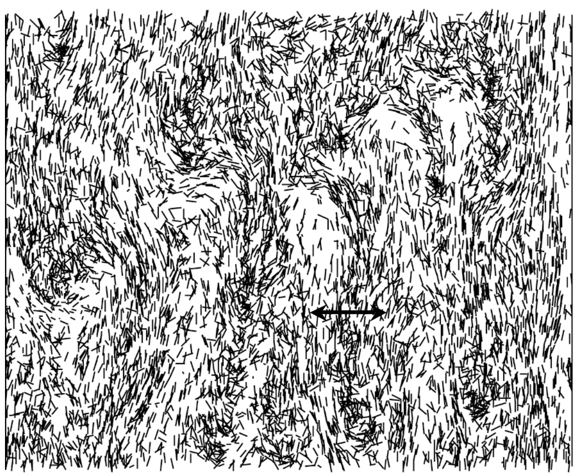
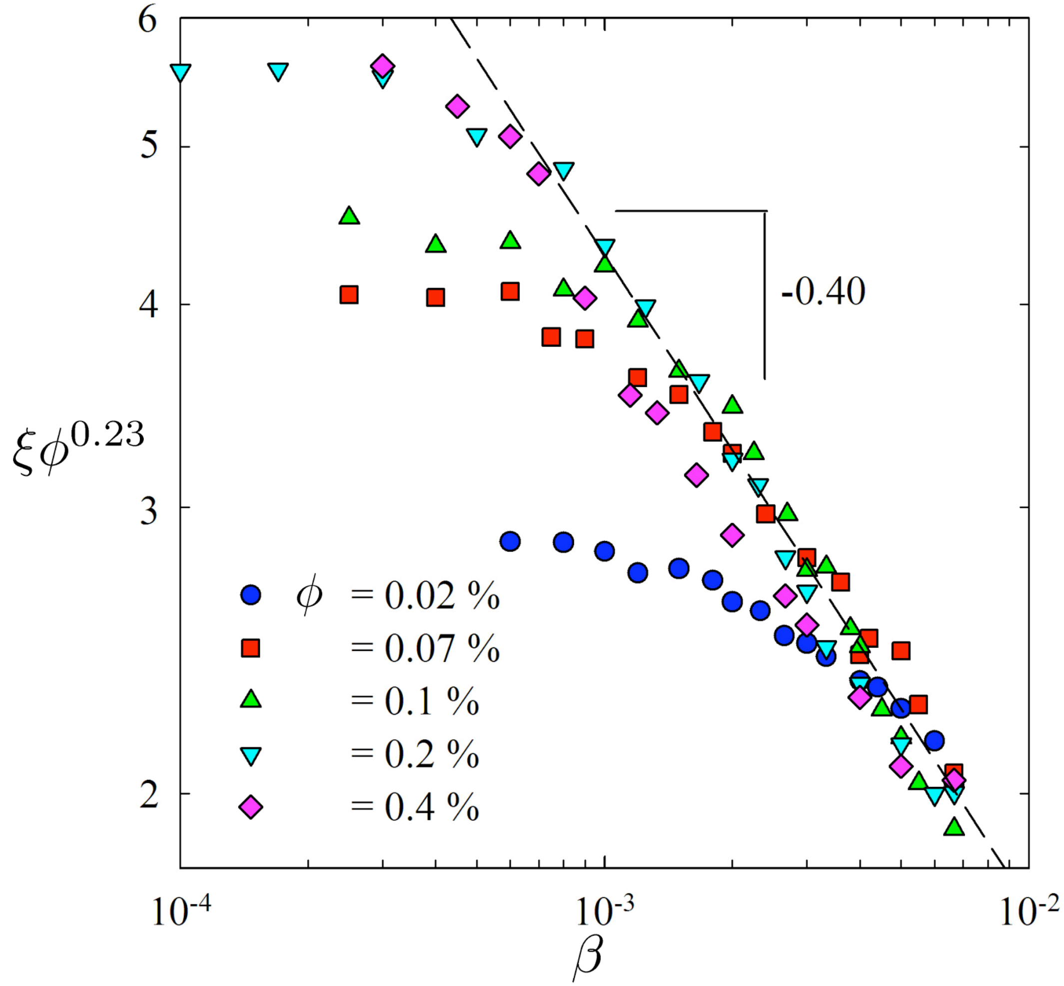
Stratification and wavenumber selection





Scaling for the correlation length:

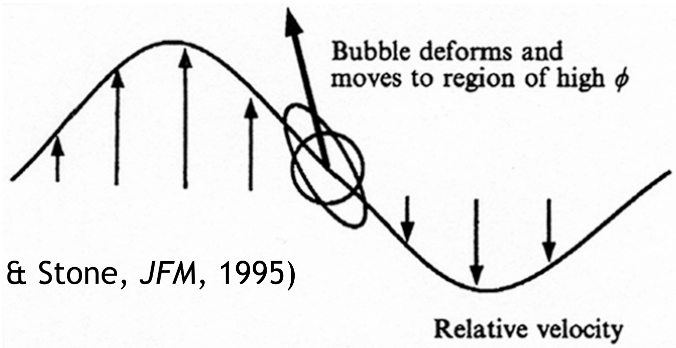
$$\xi \approx C\phi^{-0.23}\beta^{-0.40}, \quad C \approx 0.3$$



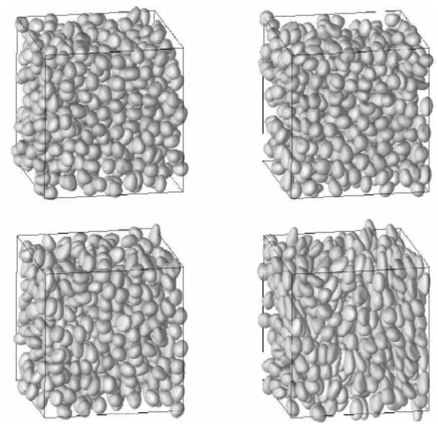
Saintillan, Shaqfeh & Darve, *Phys. Fluids* **18** 121503 (2006)

Sedimentation of deformable particles

Flow-induced deformations in non-neutrally buoyant suspensions of drops or bubbles may lead to a similar concentration instability.



(Manga & Stone, *JFM*, 1995)

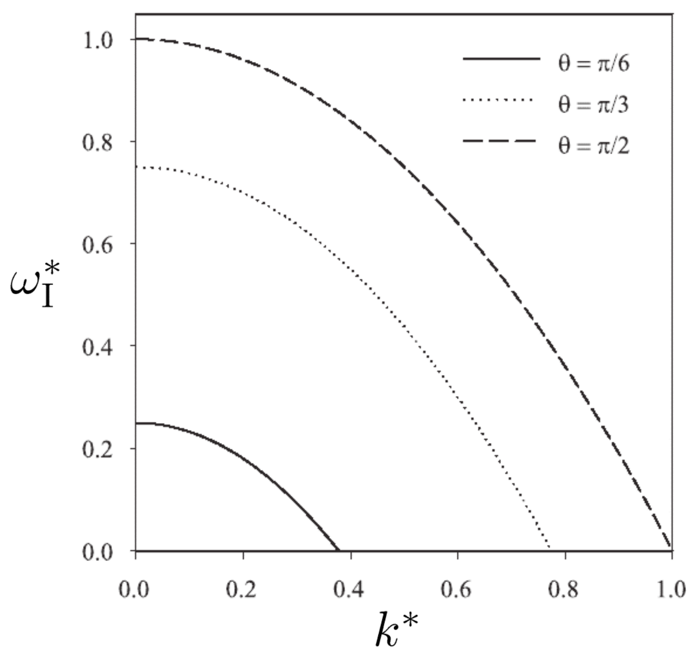


(Zinchenko & Davis, *Phil. Trans. R. Soc. Lond.* A, 2003)

Stability analysis based on:

- **Dilute suspension:** near-field interactions can be neglected.
- **Instantaneous shape relaxation:** particle shape is entirely determined by the local rate of strain.
- **Weak flow** or **small deformations:** surface tension dominates flow-induced deformations.

$$\omega_{\mathrm{I}} = \frac{\tau_s \phi M_0 F^2}{2\mu} \sin^2\theta - k^2 \left(D_{\|} \cos^2\theta + D_{\perp} \sin^2\theta \right)$$



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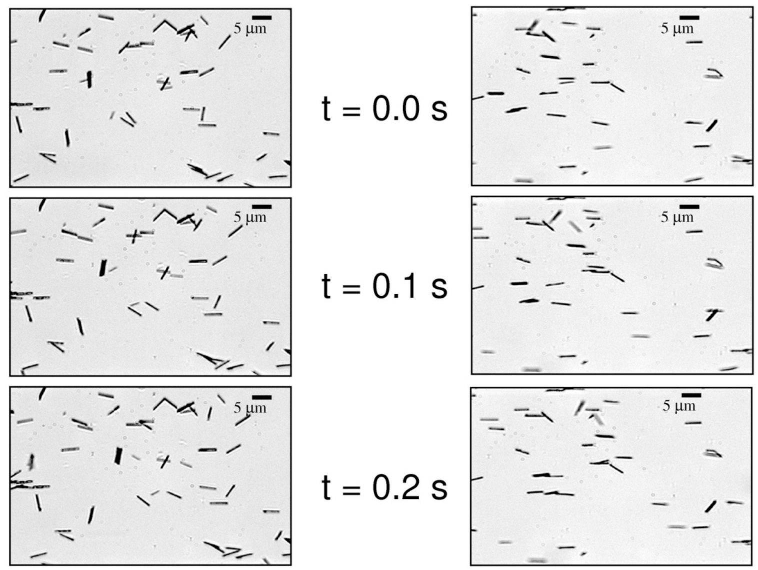
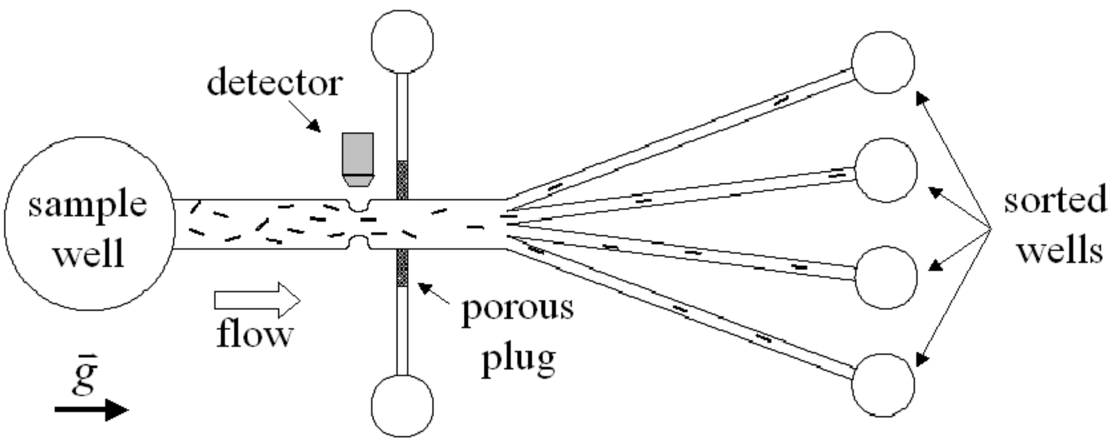
Nonlinear electrokinetics in rod suspensions

- Metallic rodlike particles are used in microfluidic devices as **"barcodes" for the detection of specific biomolecules**[1].

A nano-barcode

(Images courtesy of K. Rose and J Santiago)



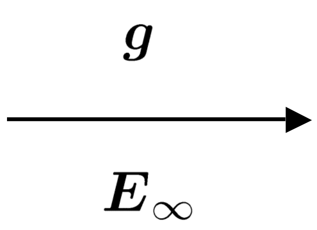


Project in collaboration with the Santiago Microfluidics Laboratory, Stanford University.

[1] Nicewarner-Pena et al., *Science* 2001.

Particle pairings

Sedimentation in an electric field shows **particle pairings**

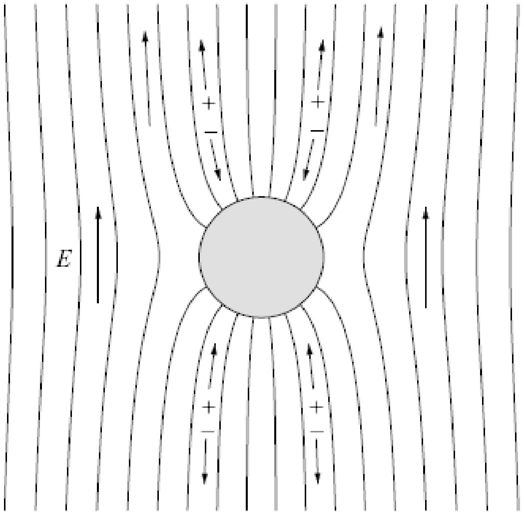


(Movie courtesy of K. A. Rose and J. G. Santiago, Stanford)

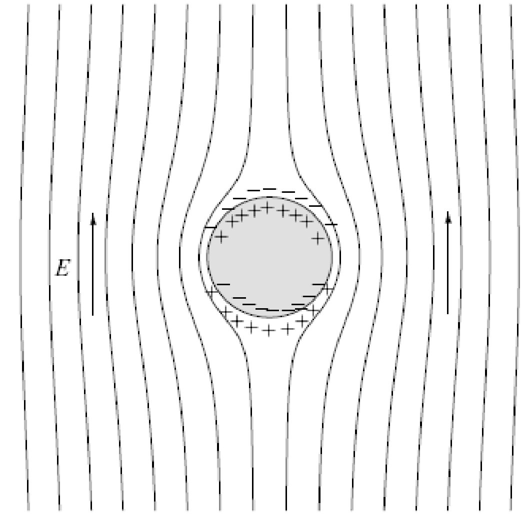
Induced-charge electrophoresis: overview

Bazant & Squires, *Phys. Rev. Lett*. 2004

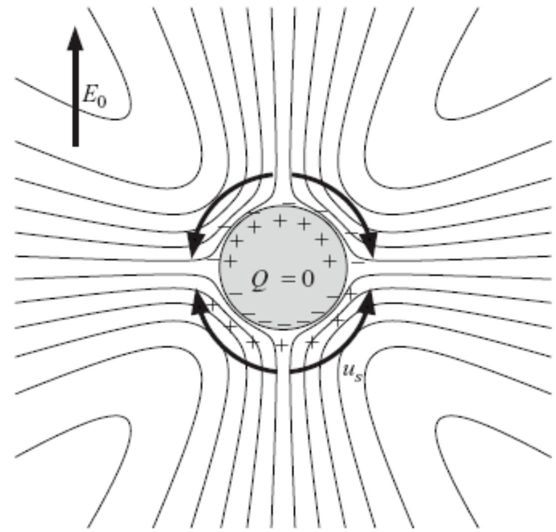
Squires & Bazant, *J. Fluid Mech*. 2004, 2006



(electric field lines)



(electric field lines)



(fluid flow streamlines)

A polarizable particle in an electric field attracts **counterions**, that accumulate near its surface, forming a **non-uniform electric double layer** (EDL).

At steady state, the particle and its EDL behave like an **insulator**. Electric potential satisfies:

$$\nabla^2 \Phi = 0$$

$$\begin{cases} \boldsymbol{n} \cdot \boldsymbol{\nabla}\Phi = 0 & \text{as } \boldsymbol{r} \in \partial S \\ \boldsymbol{\nabla}\Phi \to -\boldsymbol{E}_\infty & \text{as } r \to \infty \end{cases}$$

Potential drop across the EDL **modifies the ζ-potential**:

$$\zeta = \zeta_0 - \Phi_s$$

A fluid flow (solution of the Stokes equations) is driven by the slip on the surface:

$$\boldsymbol{u}_s = -\frac{\epsilon \zeta}{\mu} \boldsymbol{E}_s$$

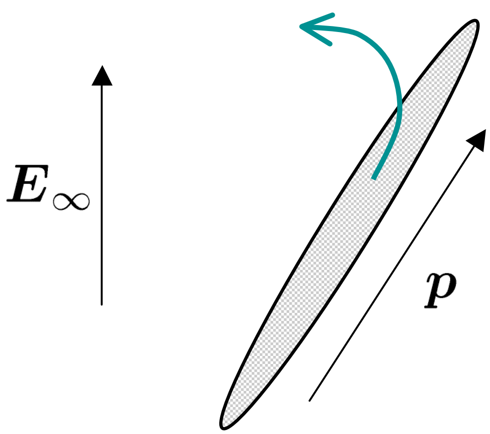
Slender-body formulation for rod-like particle

- **Electric problem solved exactly for a single spheroid**: $\begin{cases} \Phi_s = -\,\boldsymbol{x}\cdot\mathbf{G}\cdot\boldsymbol{E}_\infty \\ \boldsymbol{E}_s = (\mathbf{I}-\boldsymbol{nn})\cdot\mathbf{G}\cdot\boldsymbol{E}_\infty \end{cases}$
- **Infer slip velocity to be used in slender-body theory for rod/fluid motions:**

$$\tilde{\boldsymbol{u}}_s(s) \approx -\frac{\epsilon}{\mu} s \left(\boldsymbol{p}\cdot\tilde{\boldsymbol{E}}_\infty\right)\tilde{\boldsymbol{E}}_\infty \quad \text{where} \quad \tilde{\boldsymbol{E}}_\infty = \left[G_\parallel \boldsymbol{pp} + \frac{1}{2}G_\perp(\mathbf{I}-\boldsymbol{pp})\right]\cdot\boldsymbol{E}_\infty$$

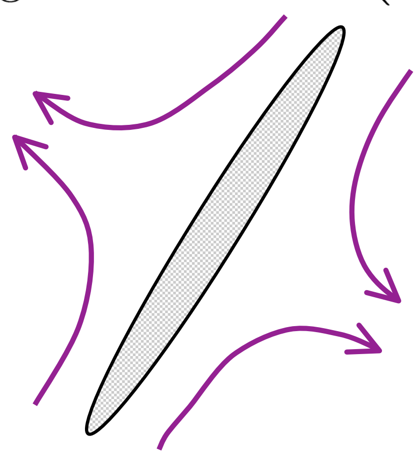
The component normal to the rod causes **alignment of the rod with the field**, at the angular velocity:

$$\boldsymbol{\Omega} = \frac{\epsilon}{\mu}\left(\boldsymbol{p}\times\tilde{\boldsymbol{E}}_\infty\right)\left(\boldsymbol{p}\cdot\tilde{\boldsymbol{E}}_\infty\right)$$



The component tangential to the rod, to leading order, **drives a stresslet flow** in the surrounding fluid, of magnitude:

$$\mathbf{S} = \frac{2\pi\epsilon l^3}{3\log 2A}\left(\boldsymbol{p}\cdot\tilde{\boldsymbol{E}}_\infty\right)^2\left(\boldsymbol{pp}-\frac{\mathbf{I}}{3}\right)$$



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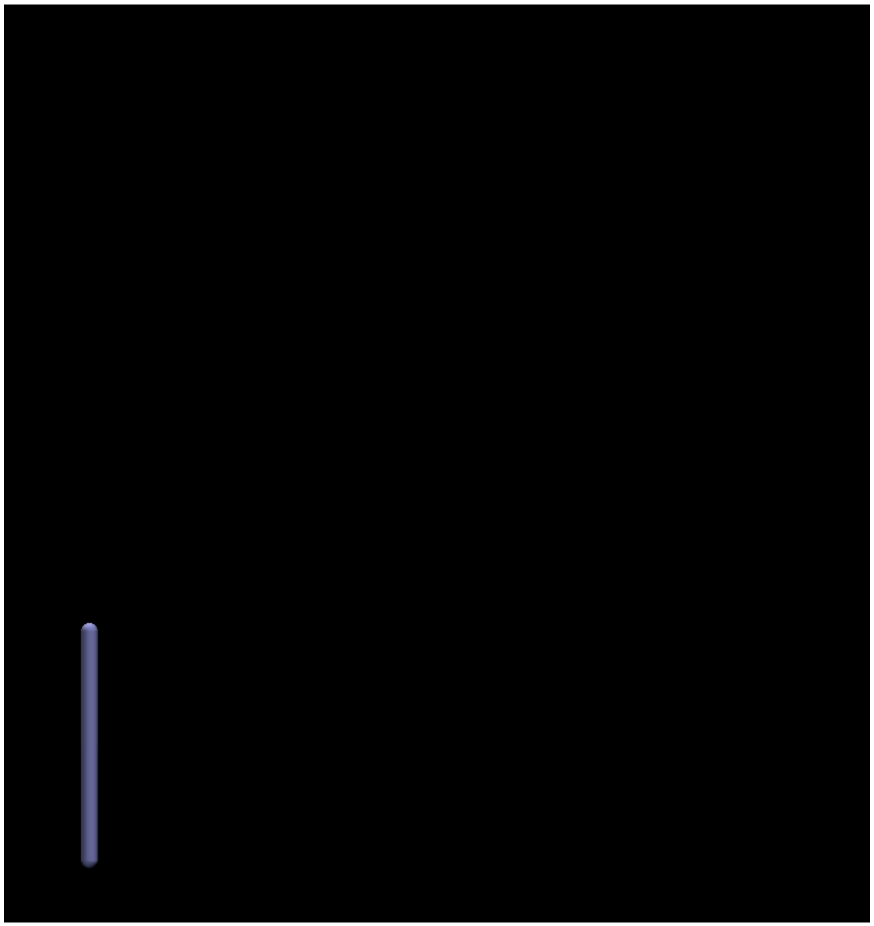
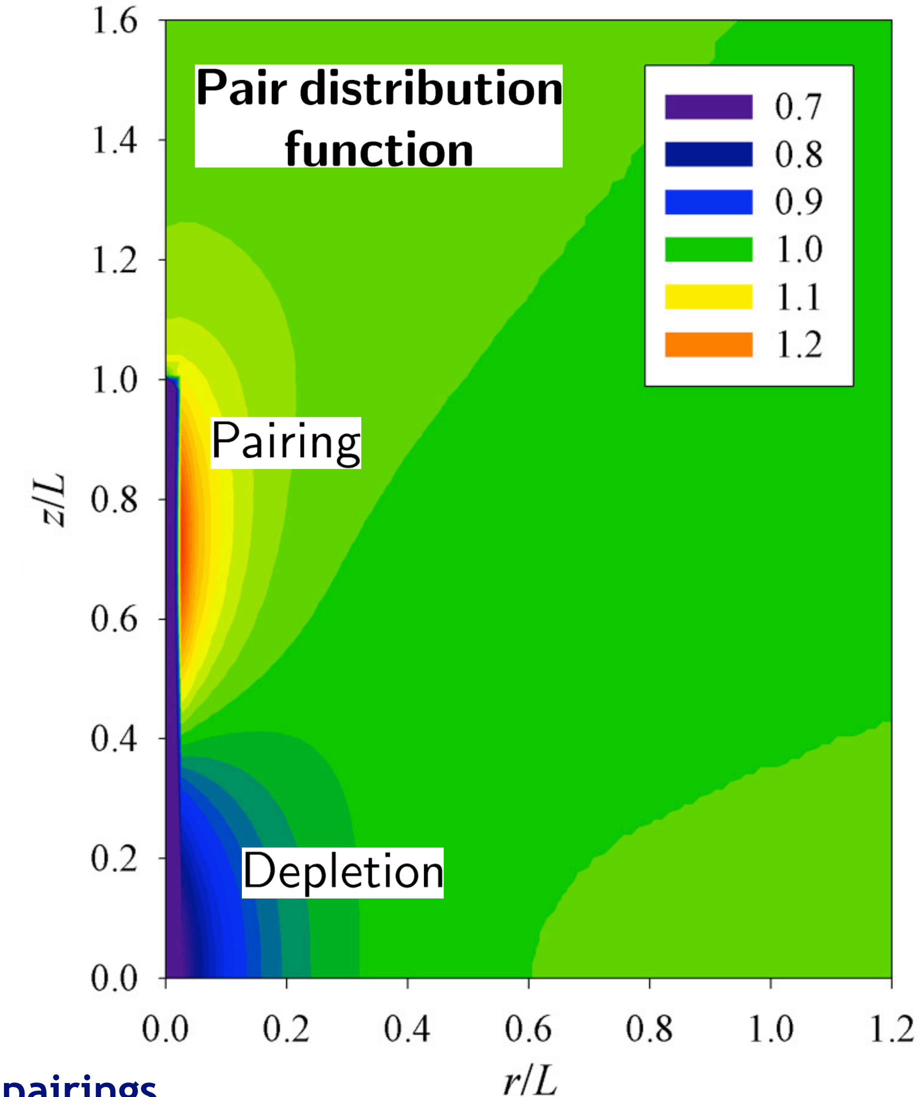
Pair interactions: semi-analytical model

- Consider two particles aligned in the z-direction. Assume a linear distribution of point-forces along their axes (stresslet interactions).
- Solve for the relative velocity analytically.

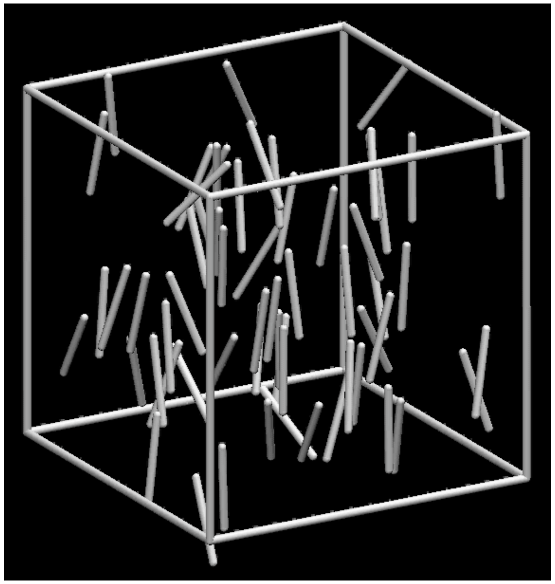




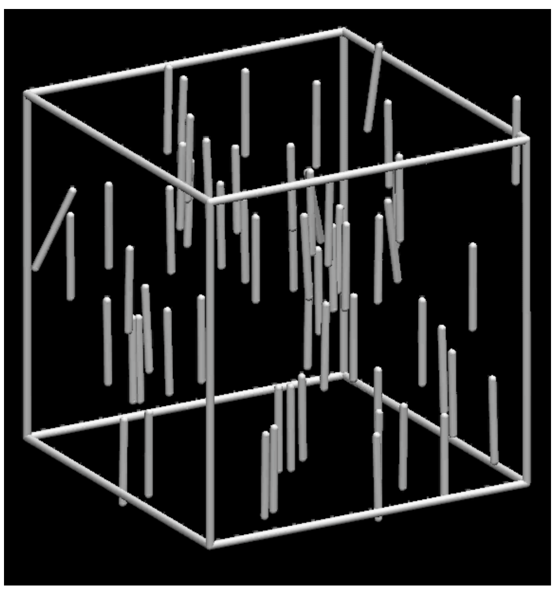
⇨ **Hydrodynamic interactions result in particle pairings**

Multiparticle simulations: Brownian systems

Pe = 10



Pe = 400



60 rods, $nl^3 = 0.1, \; A = 10$

- Simulation method includes: **far-field hydrodynamic interactions, lubrication and contact forces, ICEP slip, and Brownian motion in periodic BCs.**

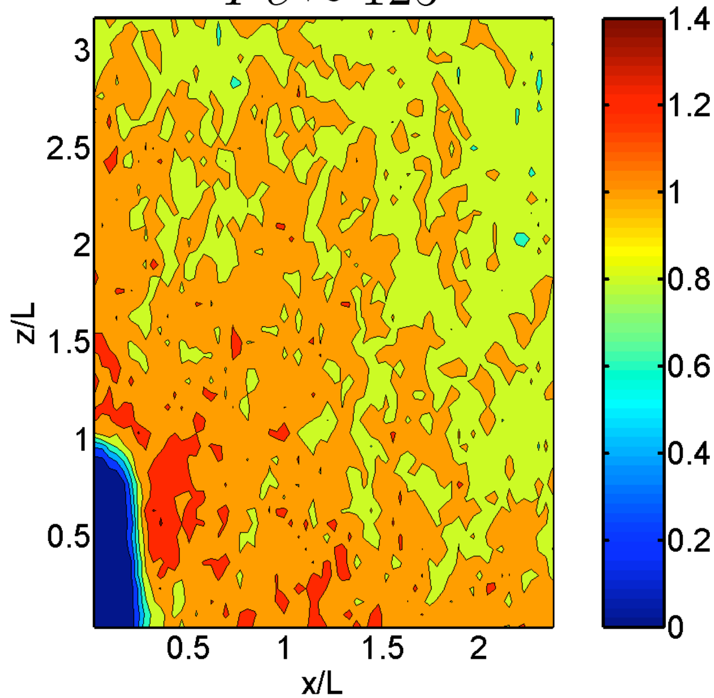
$\boldsymbol{E}_\infty$

Peclet number $$\mathrm{Pe} = \frac{\epsilon E_\infty^2}{\mu D_r} = \frac{8\pi\epsilon E_\infty^2 l^3}{3kT \log 2A}$$

Comparison to experiments

(Rose and Santiago 2006)

$Pe \approx 125$



Conclusions

- **Sedimentation of orientable particles**
  - *The sedimentation is characterized by a concentration instability*
  - *Our simulations, for the first time, captured the wavenumber selection observed in experiments.*
  - *A stability analysis suggests that stratification may be responsible for the wavenumber selection, and shows agreement with our simulation results.*
- **Induced-charge electrophoresis of polarizable rods**
  - *A model was developed for ICEP of slender rods, and used to develop an efficient simulation method for such suspensions.*
  - *Using our model, we were able to explain particle pairings obversed in experiments.*

Acknowledgments

- **Advisors:** Eric Shaqfeh (Chemical Engineering, Stanford)
  Eric Darve (Mechanical Engineering, Stanford)
- **Sedimentation:** Elisabeth Guazzelli (IUSTI, Marseille, France)
  Bloen Metzger (IUSTI, Marseille, France)
  Jason Butler (University of Florida)
  Michael Brenner (DEAS, Harvard University)
- **ICEP:** Juan Santiago (Mechanical Engineering, Stanford)
  Klint Rose (Mechanical Engineering, Stanford)
- **Funding:** Stanford Graduate Engineering Fellowship
  Gerald J. Lieberman Fellowship
  Canon Corporation