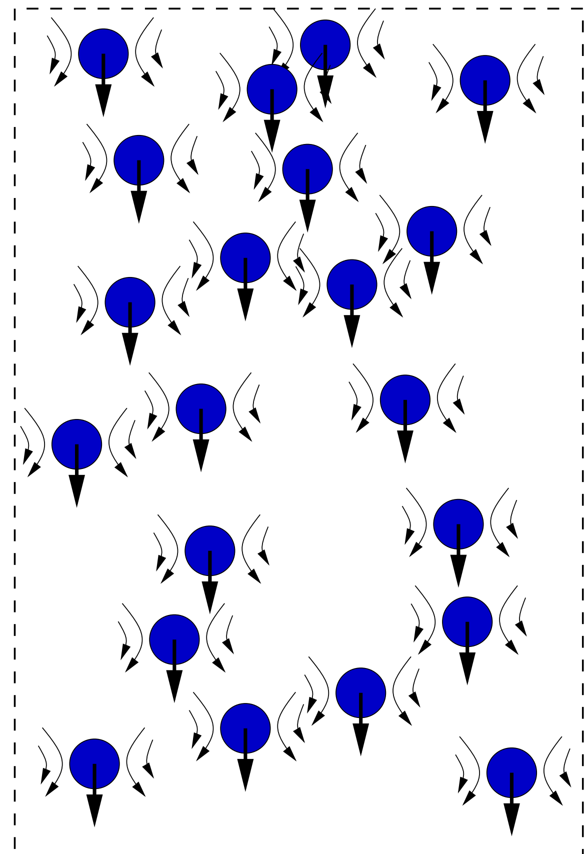
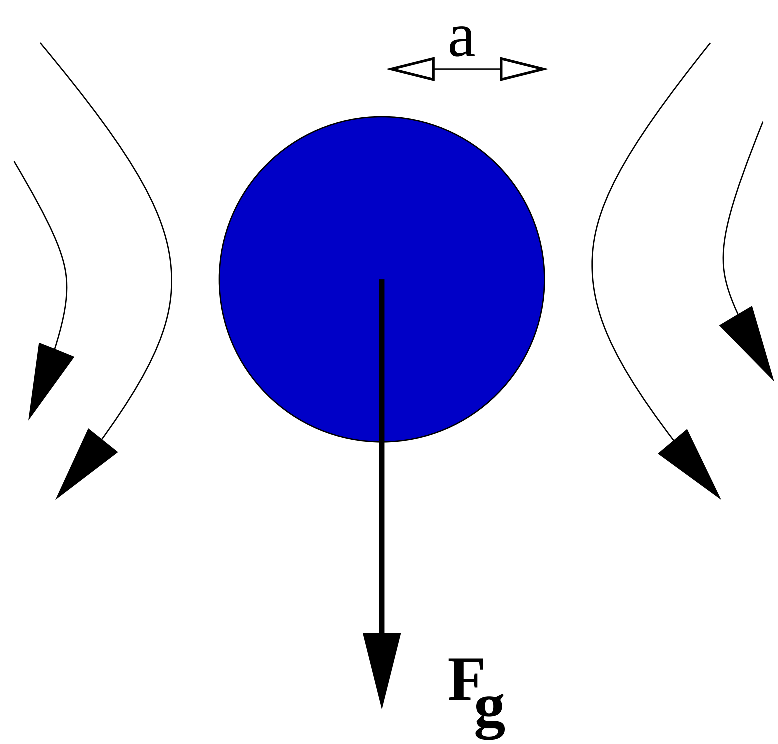
Fluctuations and Structures in Dilute Sedimentation

Peter J. Mucha, Michael P. Brenner, MIT
Boris I. Shraiman, Bell Labs
Support from NSF

- One Sphere, Two Spheres,
  Three Spheres, More...
- Fluctuations
- Simulation of Dilute Limit
- Positions, Velocities, and Densities
- Comparison with Experiment



Fluid Flows Due to Falling Sphere



$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\, \mathbf{v} = -\frac{1}{\rho}\nabla p + \frac{\mu}{\rho}\nabla^2 \mathbf{v}$$

quasi-steady Re $\ll 1$

Reynolds Number $Re = \frac{\rho V_0 a}{\mu}$

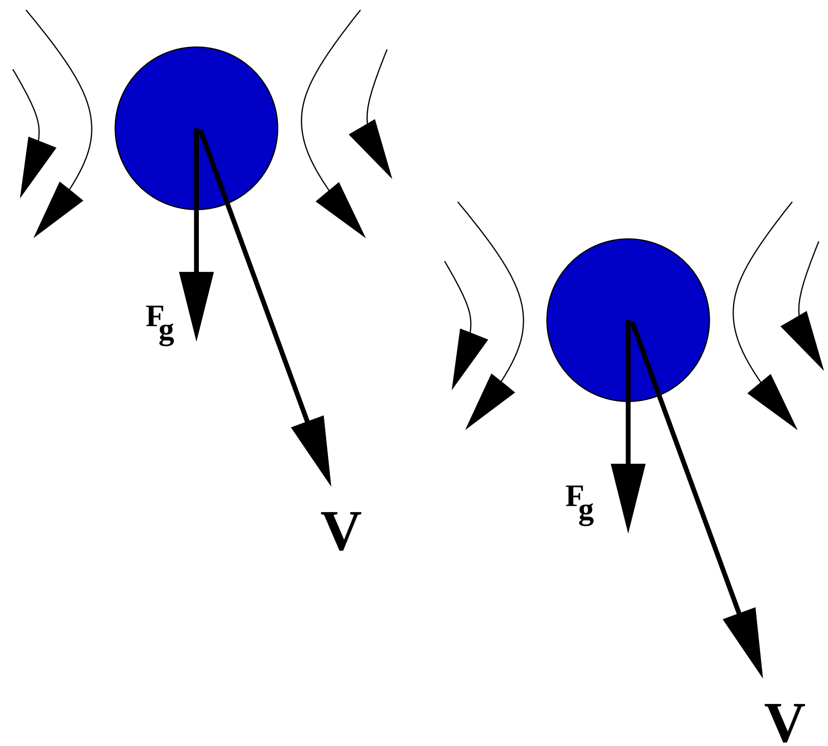
Drag balances Gravity

$m\vec{g} = 6\pi\mu a \vec{V}_0$

Quickly reaches terminal (Stokes) velocity $\vec{V}_0$ and drags fluid

$$\mathbf{v} = \vec{V}_0 \left[\frac{3a}{4r} + \frac{a^3}{4r^3}\right] + \vec{V}_0 \cdot \hat{r}\hat{r} \left[\frac{3a}{4r} - \frac{3a^3}{4r^3}\right]$$

Two Identical Spheres



Solve Stokes equations via
Bi-spherical coordinates,
Boundary Integrals, or Reflections

Each particle advects the other
Reversibility + Symmetry ⇒ Same $\vec{V}$
If $a \ll R$,

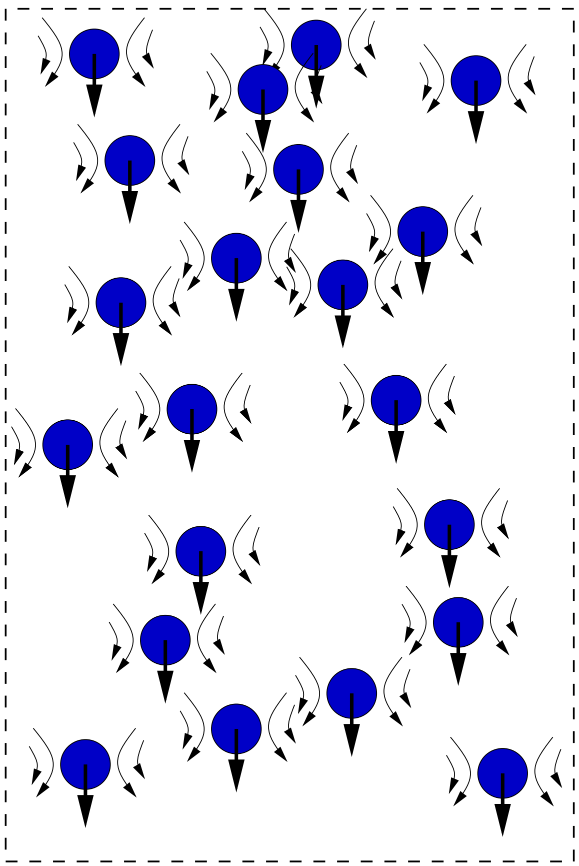
$$\vec{V} = \vec{V}_0 + \frac{3a}{4R}\left[\vec{V}_0 + \vec{V}_0 \cdot \hat{R}\hat{R}\right]$$

Three Identical Spheres yields more complicated behavior

Sensitive dependence on initial conditions [Jánosi *et al.* 1997]

Horizontally-projected area conserved [Hocking 1964]

N Identical Spheres



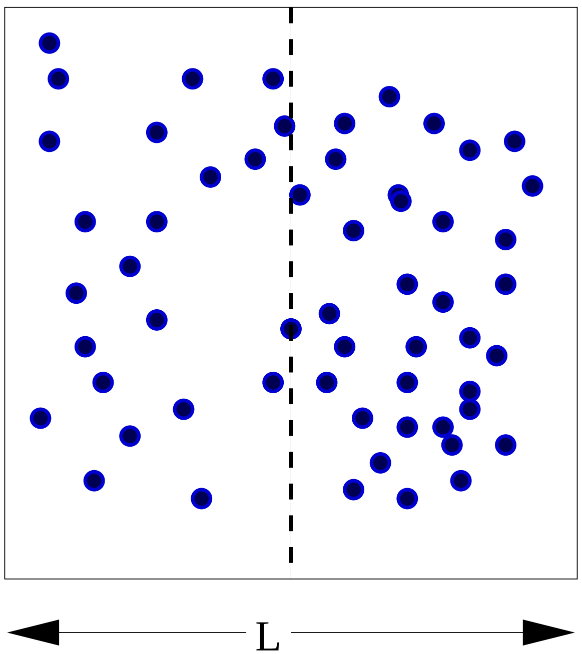
Cloud (radius A) of N particles in clear fluid cooperate: $\langle V \rangle = Nmg/4\pi\mu A = 3V_0A^2/2a^2$.

But uniformly distributed particles in vessel with bottom gives backflow, hinders settling.

Difficulty: **Long Range Interaction**
Smoluchowski (1912), Burgers (1942), Batchelor (1972), $\langle V \rangle / V_0 = 1 - 6.55c + O(c^2)$

Batchelor calculation assumes (i) random particle distribution, (ii) no side wall effects, (iii) only two-particle interactions at $O(c)$.

Density and Velocity Fluctuations



N particles. $n = N/L^3$. $c = \frac{4\pi}{3}a^3 n$.

Caflisch & Luke (1983):

$\sqrt{N}$ fluctuations $\Rightarrow$ convection current

$\sqrt{\langle \delta V^2 \rangle} \sim \sqrt{N} mg/6\pi\mu L \sim V_0\sqrt{cL/a} \sim aV_0\sqrt{nL}$

Observed Numerically [Ladd 1996]

Saturate Experimentally [Segrè 1997]

Effective Continuum Equations [Kynch 1951]:

$$\nabla p = \mu \nabla^2 \mathbf{v} + c\mathbf{f}\,, \qquad \nabla \cdot \mathbf{v} = 0\,, \qquad \frac{\partial}{\partial t}c + (\mathbf{v}\cdot\nabla)c = D\nabla^2 c\,.$$

What sets D?

Missing macroscopic variables to describe fluctuations?

Numerical Simulation of Hydrodynamic Interaction

Have to handle Long Range Interactions

In general, complicated hydrodynamics (no slip every particle):
Stokesian Dynamics [Brady 1985], FMM [Sangani 1996],
P^3M [Higdon], Lattice-Gas [Ladd 1994]

Dilute Point-Force Interactions much easier:

$$\vec{V}^{(i)} = \vec{V}_0 + \sum_{j \neq i} \frac{3}{4} a \vec{V}_0 \cdot \left[\frac{1}{R^{(ij)}} \left(\mathbf{I} + \hat{R}^{(ij)} \hat{R}^{(ij)} \right) \right]^{BC} + \text{shortrange}$$

BC: Green's function modified by external boundary conditions

Triply-Periodic Boundary Conditions, or Doubly-Periodic with pair of Slip Side Walls, Normal Flow Side Walls, or No-Slip Walls
Ewald Summation, no $k = 0$ mode ($\langle \vec{v} \rangle = 0$)

P^3M: *Long-Range by FFT, correct direct int's locally*

Consider Well-Separated Particles in Dilute Limit

Keep only r^{-1} terms – *Point-Force Interactions*

$$\vec{V}^{(i)} = \vec{V}_0 + \sum_{j \neq i} \frac{3}{4} a \vec{V}_0 \cdot \left[\frac{1}{R^{(ij)}} \left(\mathbf{I} + \hat{R}^{(ij)} \hat{R}^{(ij)} \right) \right]$$

Does a Matter?

In self-velocity frame, a and V_0 only appear as product

$$D_0 = aV_0 \sim F_0/\mu \,.$$

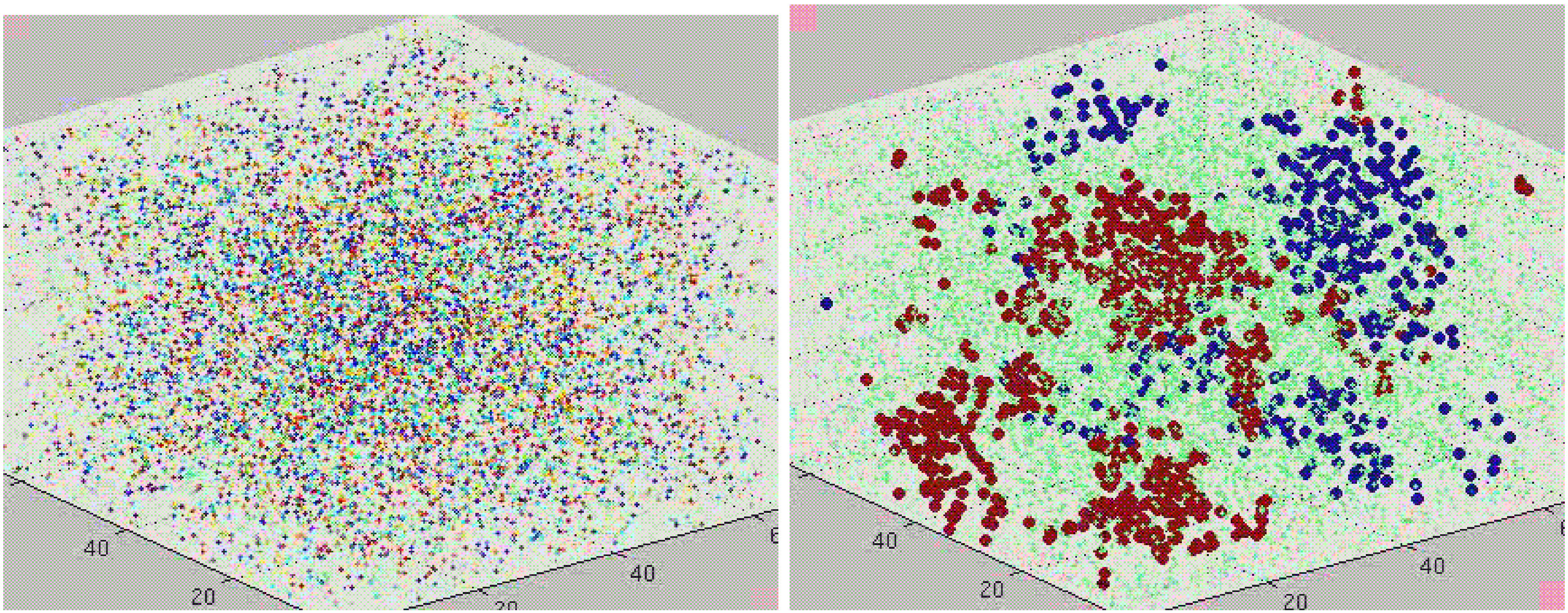
$\Rightarrow$ Configurational changes $\sim f(n = N/L^3,\, L,\, D_0 = aV_0,\, t)$

Caflisch-Luke $\sqrt{\langle \delta V^2 \rangle} \sim D_0 \sqrt{nL}$

Macroscopic Diffusion Coefficient $\sim D_0 \tilde{f}(N)$

No Stokes Time (a/V_0), Time scale $\sim L/\langle \delta V^2 \rangle^{1/2}$

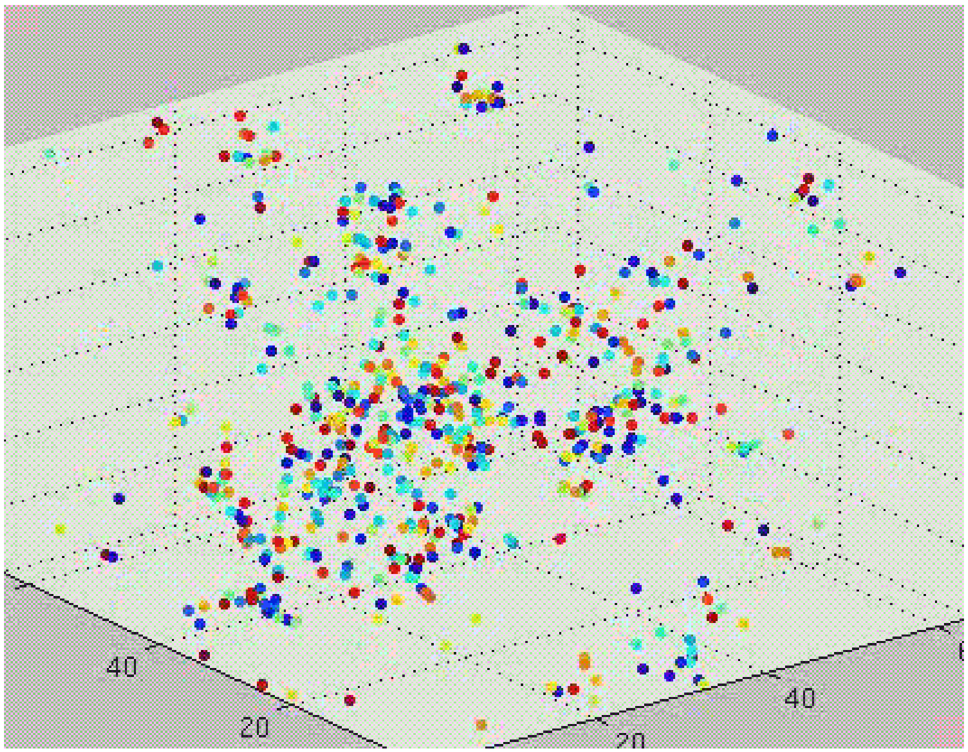
Simulation Results

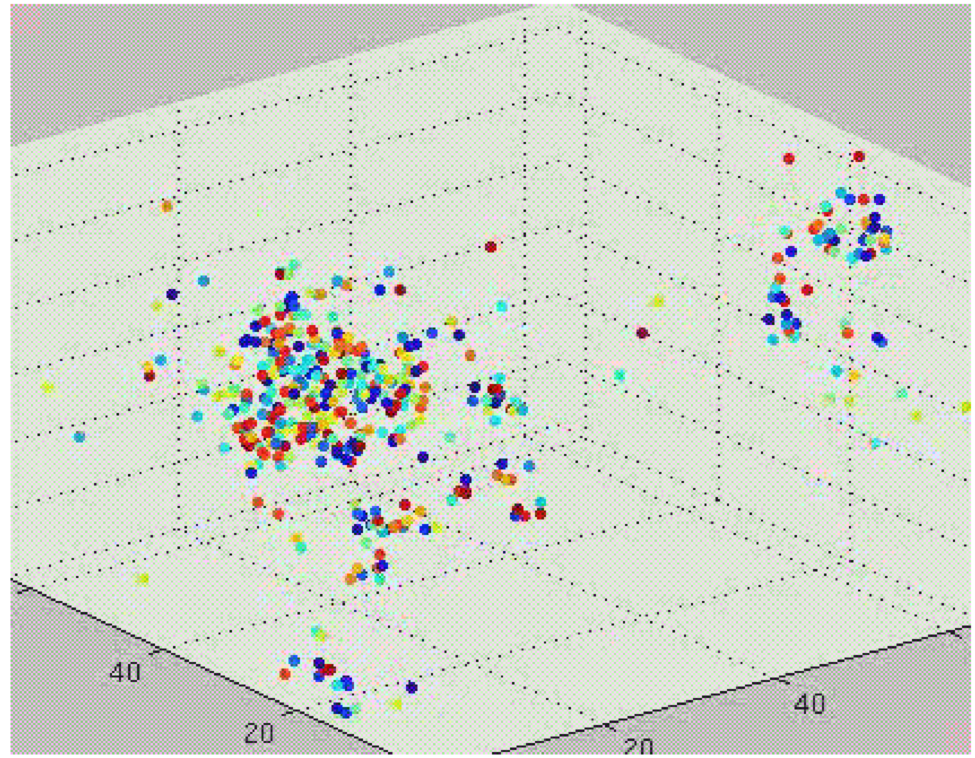


LEFT: *Every particle individually colored*

RIGHT: 1.5σ *fast*, 1.5σ *slow*

Fastest Moving Particles



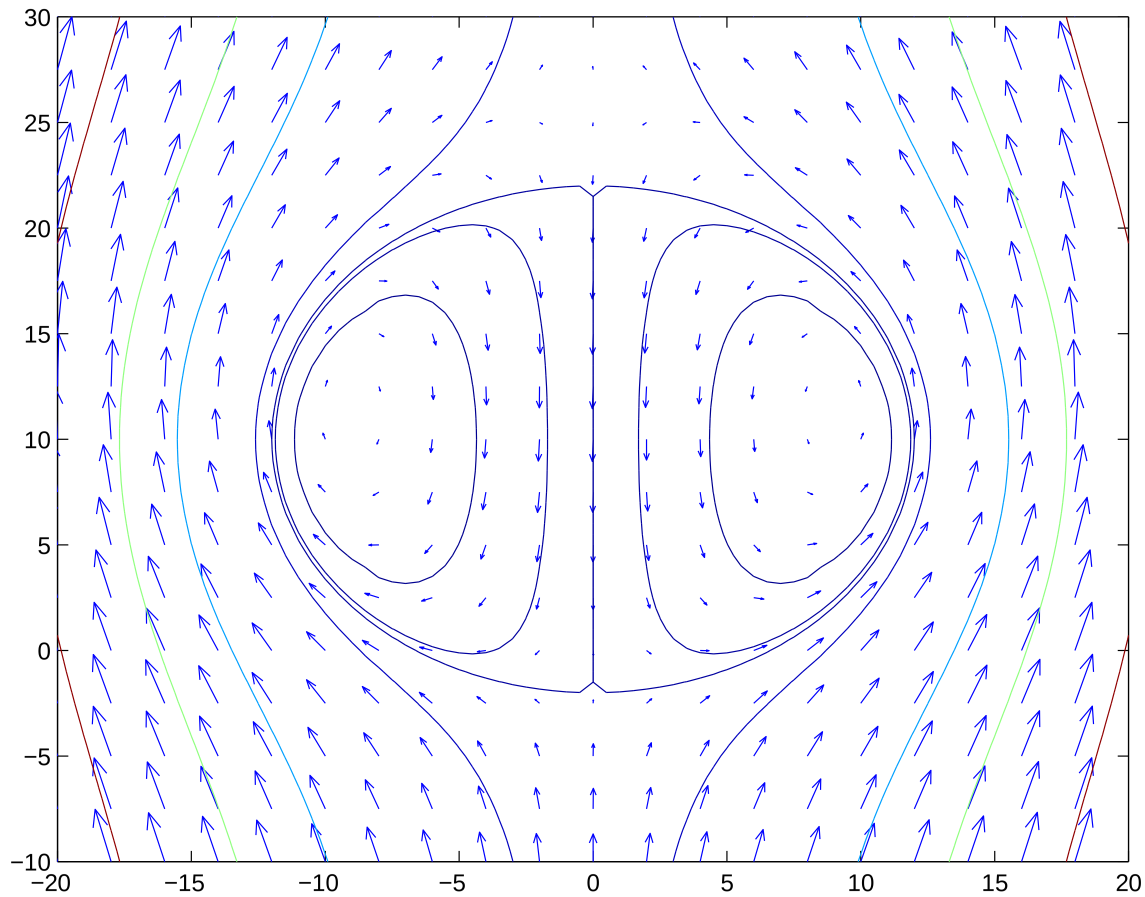


Individually color 2.5σ fast particles w/ time window

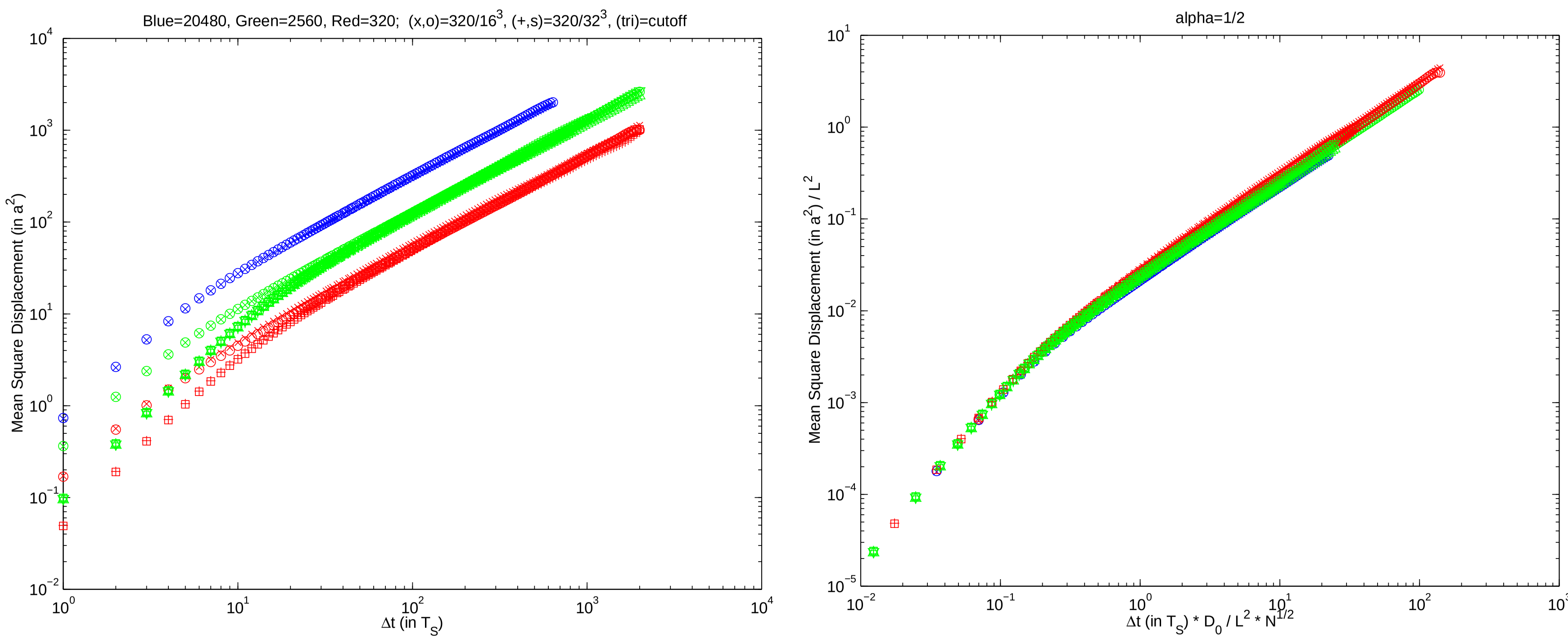
LEFT: Collection of small "blobs"
RIGHT: System dominated by one large blob

Blobs look like Hadamard solution

Heavy fluid in light fluid



Hydrodynamically-Induced Diffusion



CL plus $T \sim L/\sqrt{\langle \delta V^2 \rangle} \Rightarrow \langle \delta x^2 \rangle = L^2 \tilde{f}(\sqrt{N} D_0 t / L^2)$

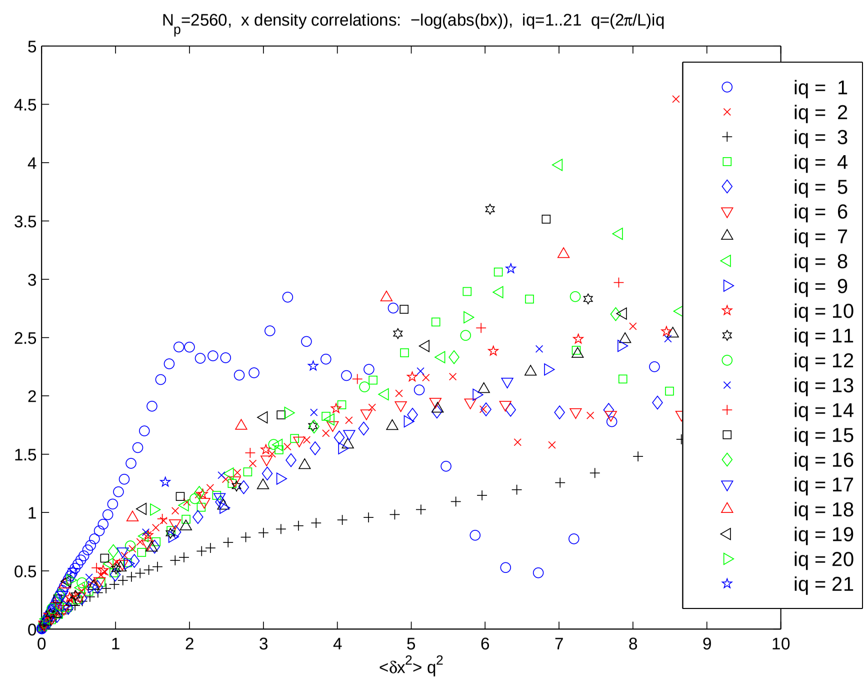
$$D_{\perp eff} \approx (0.03)\sqrt{N} D_0$$

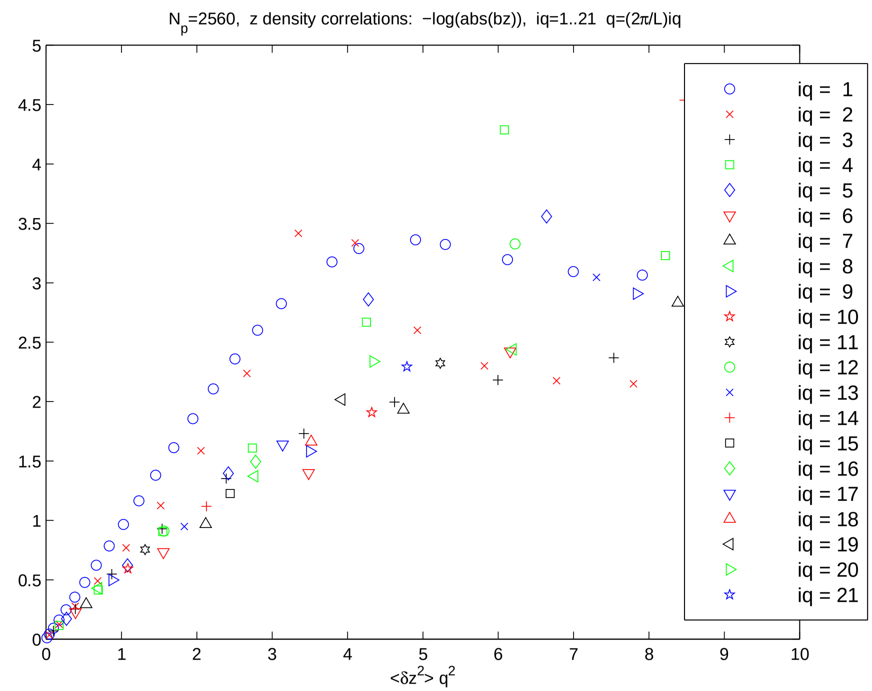
$\langle \delta z^2 \rangle$? $\langle \delta V_z^2 \rangle$ and crossover time each ~ 10 times larger

$\Rightarrow D_{\| eff} \sim 100 D_{\perp eff}$; but scaling not understood

Density Correlations $\langle \rho_{\mathbf{q}}(t_0+\Delta t)\rho_{-\mathbf{q}}(t_0)\rangle \sim \exp\{-\frac{1}{2}q^2\langle(\delta r_{\perp,\parallel})^2\rangle\}$?

Plot $-\log\langle \rho_{\mathbf{q}}(t_0+\Delta t)\rho_{-\mathbf{q}}(t_0)\rangle$ vs. $q^2\langle(\delta r_{\perp,\parallel})^2\rangle$





$\perp$ $\qquad\qquad$ $\parallel$

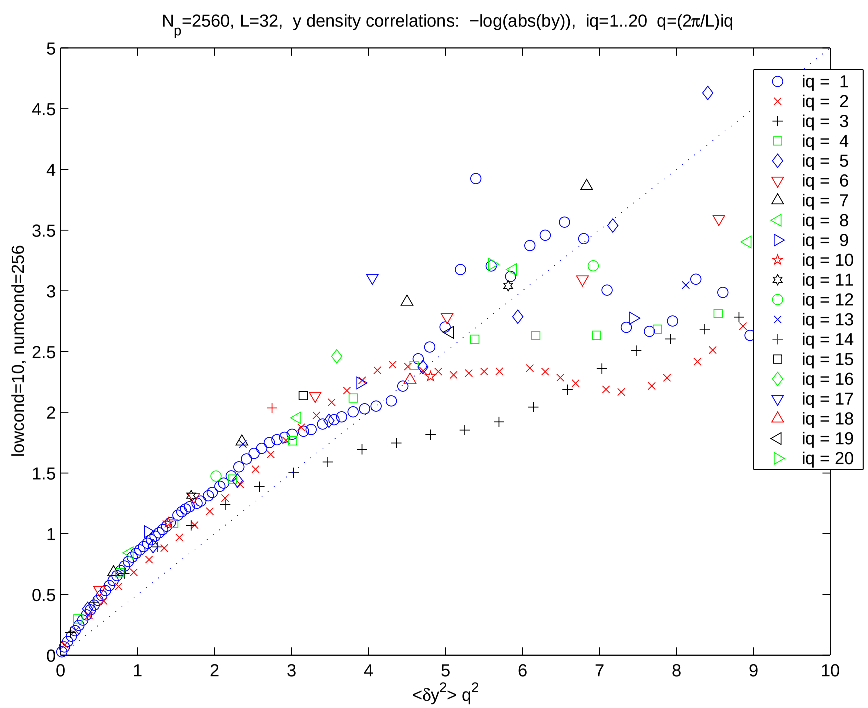
Short-time decay understood in terms of particle displacements, except for smallest q's. $\exp\{-\frac{1}{2}q^2\langle(\delta r_{\perp,\parallel})^2\rangle\} \neq \exp\{-\frac{1}{2}q^2\sigma^2t^2\}$, assuming so would give incorrect velocity fluctuations.

Agrees with experiments: S. Manley, S. Tee, D. Weitz, Harvard

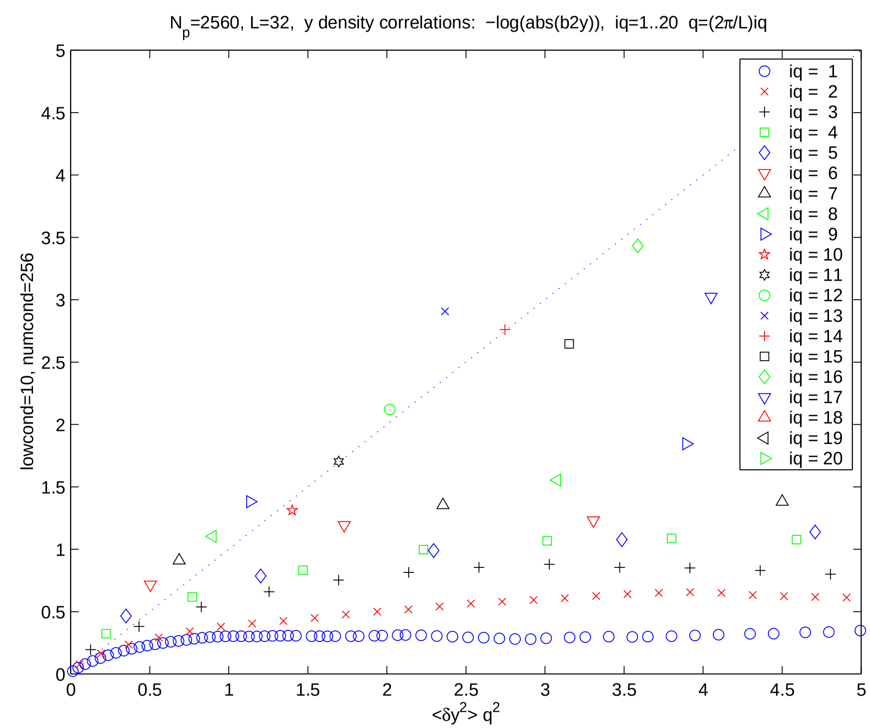
Pair Density Correlations similar (effectively independent)

Conditional Density Correlations

Plot $-\log\langle P_{\mathbf{q}}(t_0+\Delta t)P_{-\mathbf{q}}(t_0)\rangle$ vs. $q^2\langle(\delta r_{\perp,\parallel})^2\rangle$



Eulerian $\perp$



Pair $\perp$

Pair correlations conditional on being fast decay anomalously slowly $\Rightarrow$ *Long lifetime for Blob*

Summary

P^3M Simulation of Dilute Limit Microscopic Interactions

$\langle \delta r_\perp^2 \rangle$ as expected from Dilute dim'l analysis, Caflisch-Luke. $\langle \delta z^2 \rangle$?

Density Correlations accurately described by Displacements, except for smallest $\vec{q}$'s. Accurately predicts exponent $< t^2$.

Conditional Pair Correlations imply Coherence of Fast Particles.
How to incorporate blobs in effective macroscopic theory?
How to saturate Velocity Fluctuations via Blobs?