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East Rutherford, NJ
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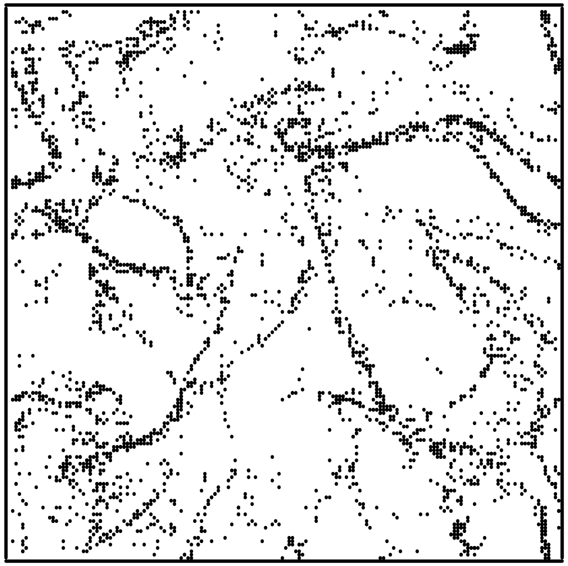
Using DNS to Understand Aerosol Dynamics

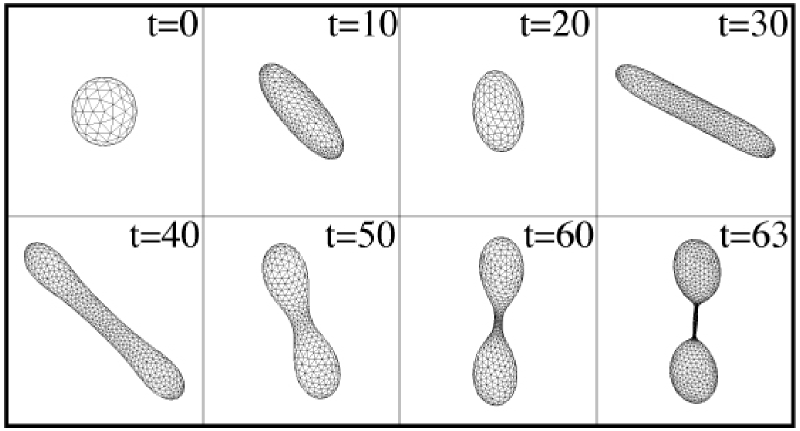
Lance R. Collins

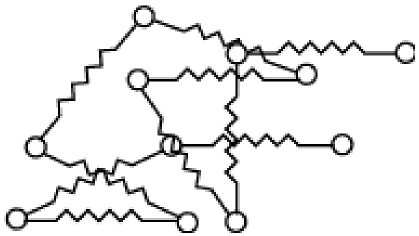
Sibley School of Mechanical & Aerospace Engineering

Cornell University

Direct Numerical Simulations of Microstructures







Aerosols
- Dispersion
- Turbulence modulation
- Coagulation

Droplets*
- Breakup
- Coalescence

* M. Loewenberg
J. Blawzdziewicz
V. Cristini

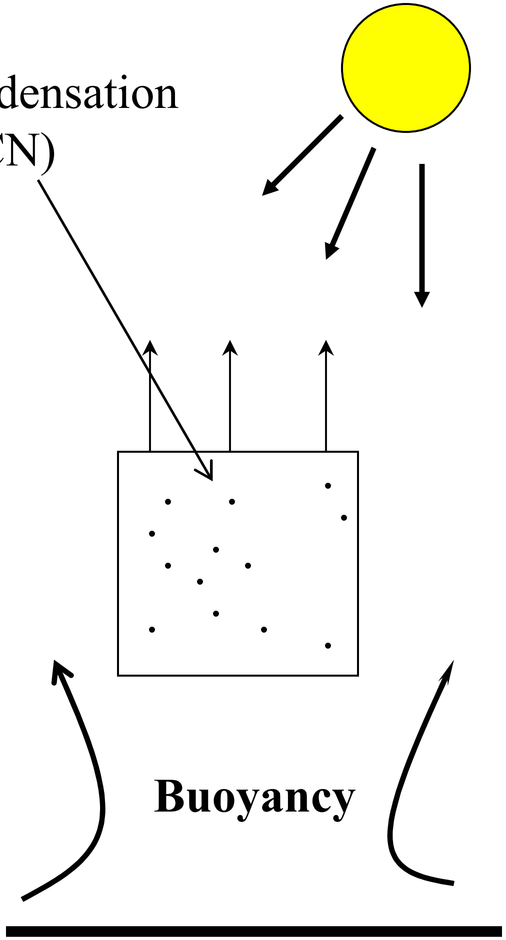
Polymer Molecules
- Orientation
- Stretch
- Drag Reduction

* J. G. Brasseur

Outline

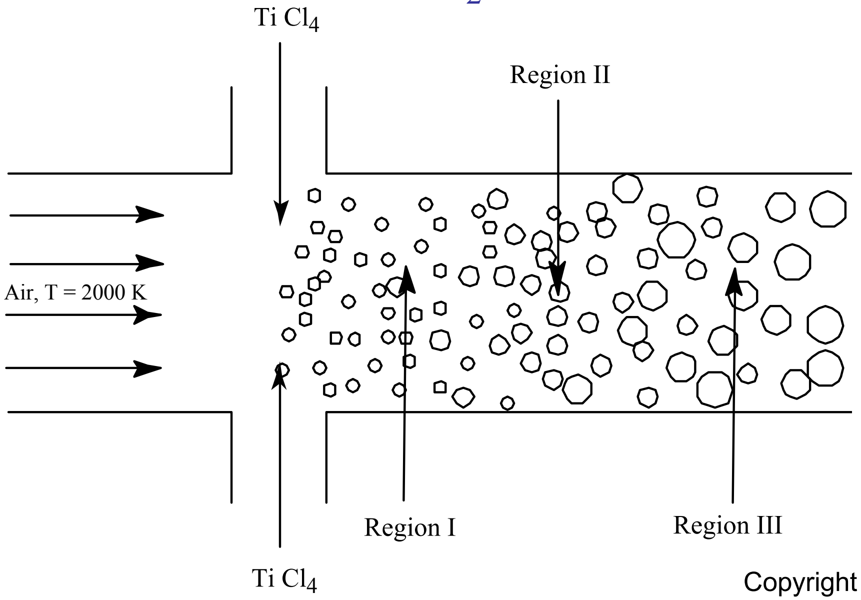
- Background on aerosols
- Direct numerical simulations (DNS)
- Numerical Results
- Theory
- Experiments
- Summary

Examples



R. Shaw, ARFM 2003

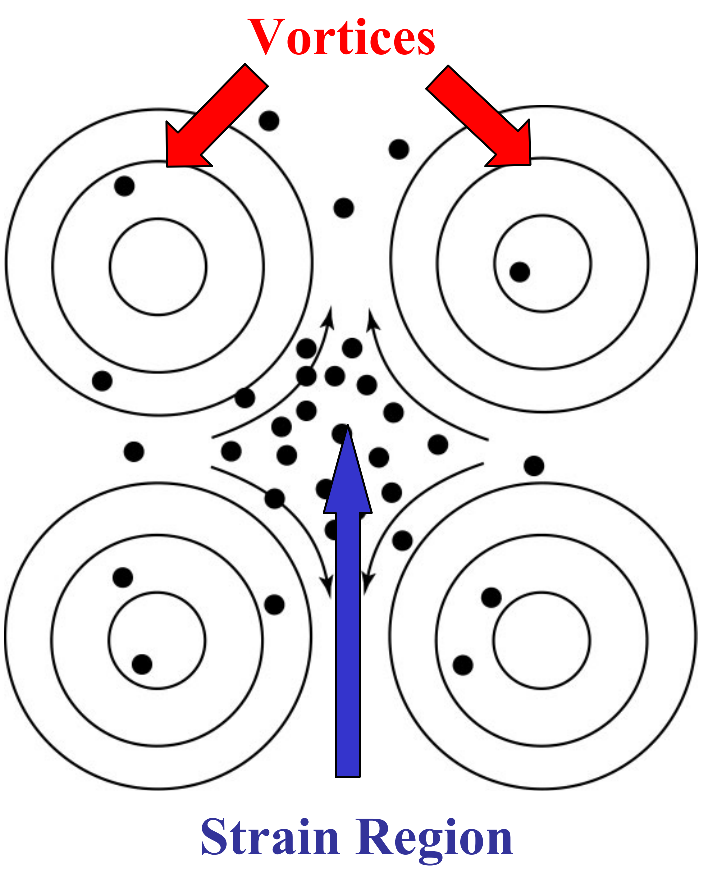
DuPont TiO_2 Process



Turbulent clustering

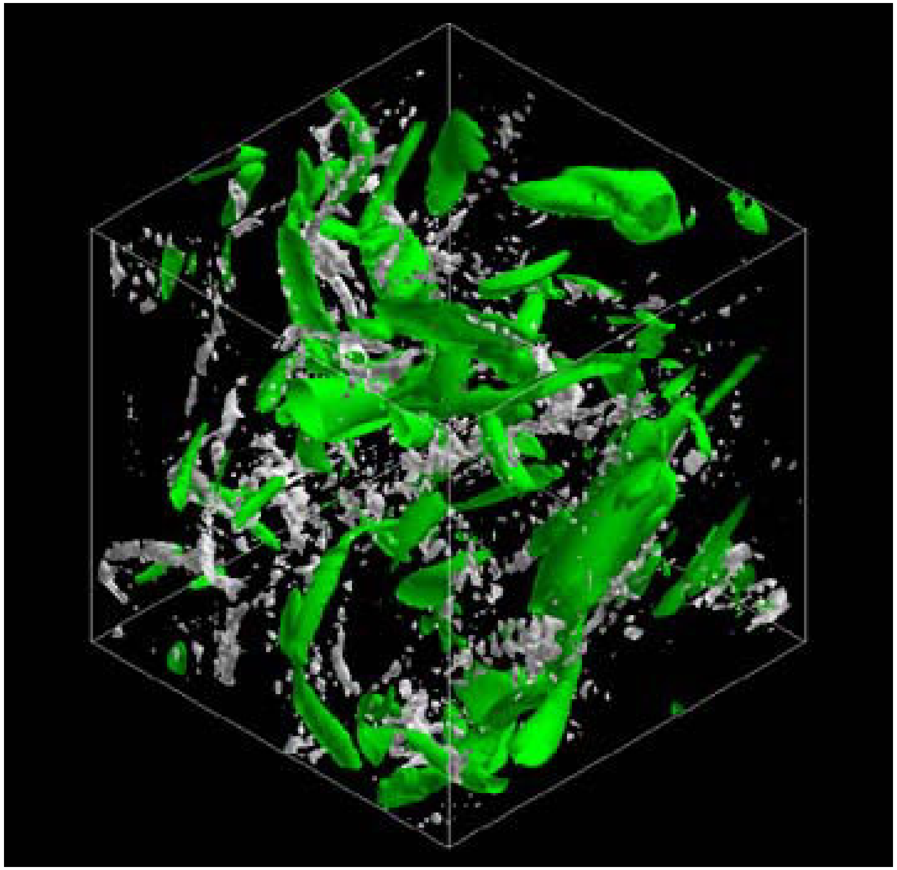
Aerosol particles in a turbulent flow field cluster outside of vortices due to a centrifugal effect, sometimes referred to as "preferential concentration."

Maxey (1987)
Squires & Eaton (1991)
Wang & Maxey (1993)



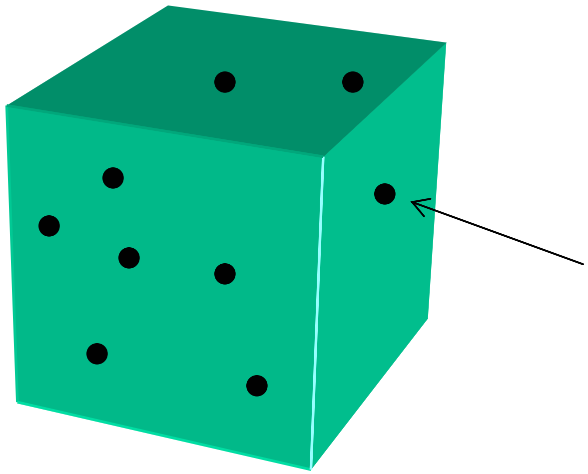
Snapshot of particle clustering in DNS

Snapshot from a DNS (St=1 and R_λ = 54). The **green tubes** are vortex tubes where fluid circulates rapidly and the **white** shows where the particle concentration is greater than 10 times the mean.



How does this affect coalescence rates?

Direct numerical simulation

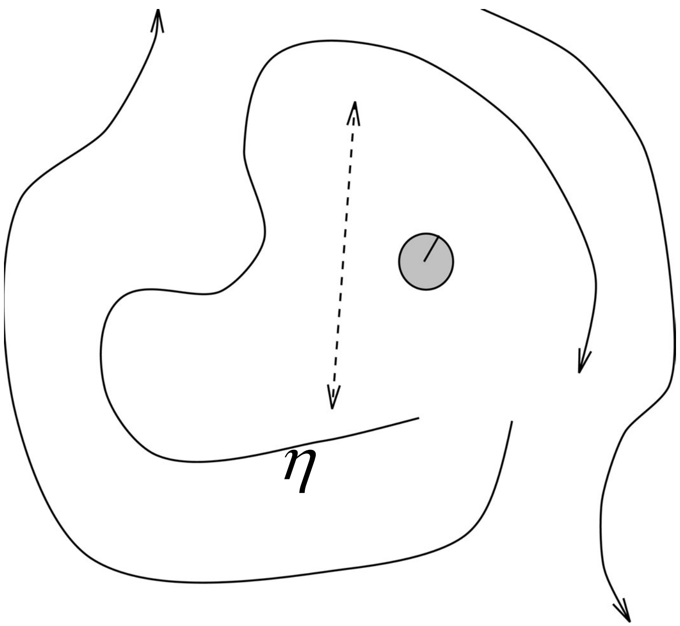


dilute loading of spheres

$$\nabla \bullet \mathbf{u} = 0$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \bullet \nabla \mathbf{u} + \frac{\nabla p}{\rho} = \nu \nabla^2 \mathbf{u} + \mathbf{F}$$

Particle update



$$\frac{d}{\eta} << 1$$

$$\frac{d\mathbf{x}_p^{(i)}}{dt} = \mathbf{v}_p^{(i)}$$

$$\frac{d\mathbf{v}_p^{(i)}}{dt} = \frac{\left[\mathbf{u}(x_p^{(i)}, t) - \mathbf{v}_p^{(i)}\right]}{\tau_p^{(i)}} + \sum_{j \neq i} \mathbf{F}^{(ij)}$$

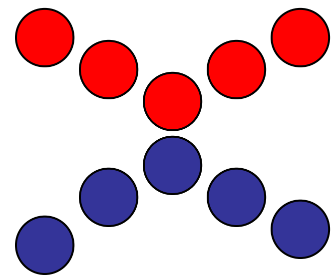
Stokes drag

collisions (neighborhood search)

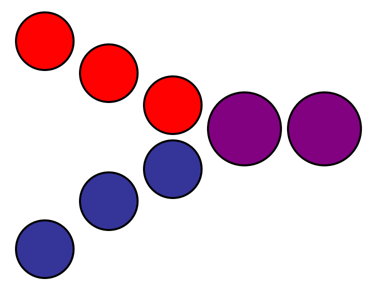
$$\tau_p^{(i)} = \frac{1}{18} \frac{\rho_p}{\rho} \left(\frac{d}{\eta}\right)^2$$

Particle-particle interactions

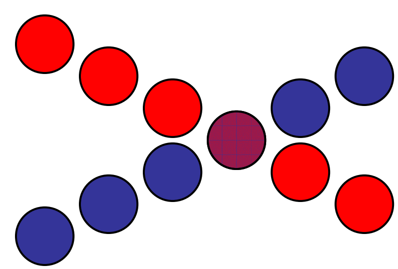
Elastic Rebound:



Coalescence:



Interpenetration:



Parameters

Flow:

U' turbulence intensity
ε dissipation rate
ν kinematic viscosity

Particles:

d diameter
ρ_p density
n loading

$$R_\lambda \equiv \sqrt{\frac{15}{\nu\,\varepsilon}}\,U'^2$$

$St = \dfrac{\tau_p}{\tau_\eta}$ Stokes number

$\dfrac{d}{\eta}$ size parameter

Φ volumetric loading

Parameter Ranges

System	R_λ	St	d/η	Φ
Clouds	10^4	$10^{-4} - 10^{-1}$	$10^{-2} - 10^{-3}$	$< 10^{-6}$
DNS	$50 - 160$ *	$10^{-2} - 1$	$10^{-2} - 10^{-1}$	$< 10^{-5}$
Exp't	$10^2 - 10^3$	$> 10^{-3}$	$10^{-2} - 10^{-1}$	$< 10^{-5}$

- **We are not able to simulate atmospheric Reynolds numbers**
- **It's therefore critical that we understand the importance of this parameter (from experiments, theory, etc.)**

* High end DNS is 4096^3, corresponding to $R_\lambda \sim 1000$
Gotoh & Fukayama (2001)

Limiting theories for collision

Saffman and Turner (1956)
Zero Stokes number:

$$N_c = \frac{1}{2} n^2 d^3 \left(\frac{8\pi}{15} \frac{\varepsilon}{\nu} \right)^{1/2}$$

Brunk, Koch & Lion (1998)
Wang, Wexler and Zhou (1998)

Abrahamson (1975)
Infinite Stokes number:

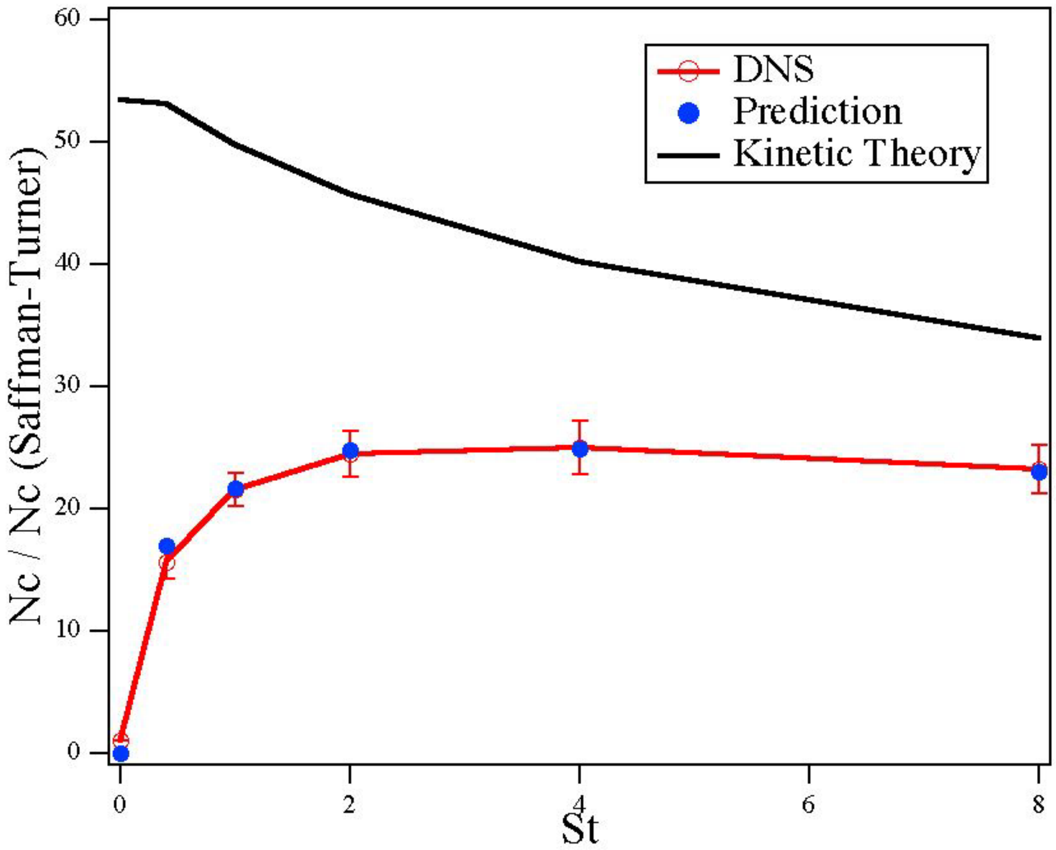
$$N_c = \frac{1}{2} n^2 d^2 \left(\frac{16\pi \, \overline{v_p^2}}{3} \right)^{1/2}$$

n number density

$\overline{v_p^2}$ particle kinetic energy

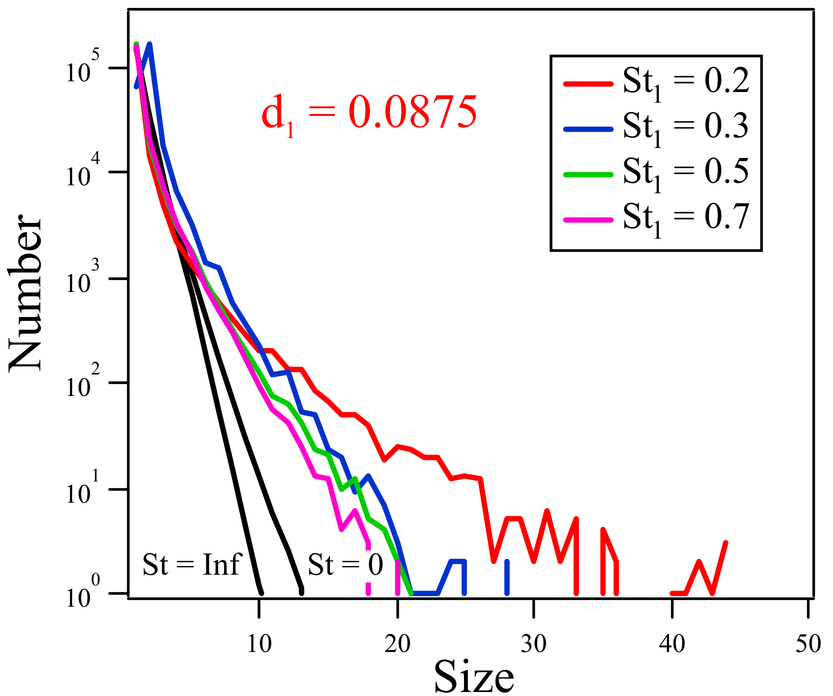
Reade & Collins (1998)

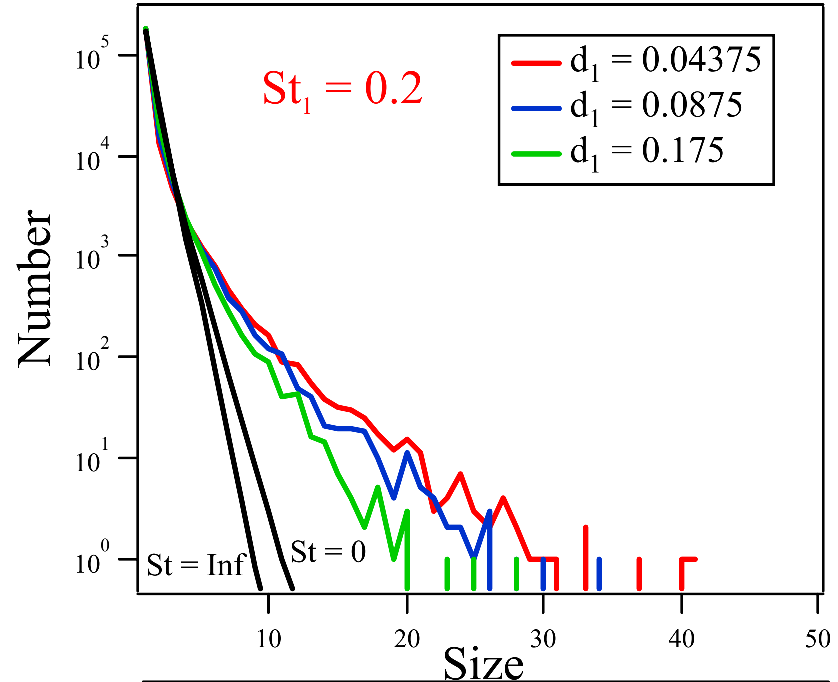
Collision vs Stokes number

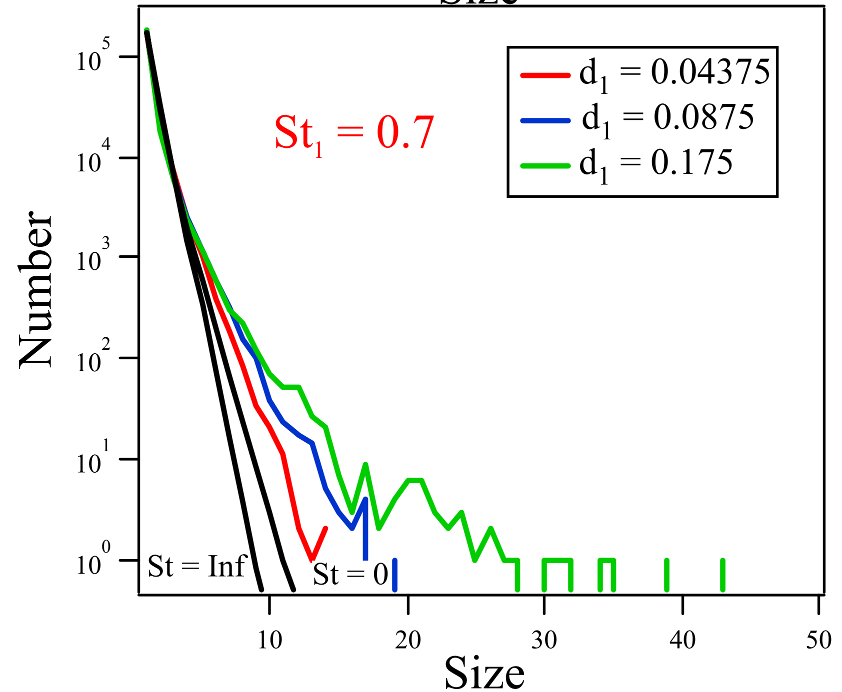


Sundaram & Collins (1997)

Evolution of size distribution







Reade & Collins JFM (2000)

General collision formula

$$N_c = \pi \, d_{ij}^2 \, n_i \, n_j \, g_{ij}(d_{ij}) \int_{-\infty}^{0} (-w) \, P_{ij}(w \,|\, d_{ij}) \, dw$$

$$\begin{aligned} d_{ij} &= (d_i + d_j)/2 \\ g_{ij}(r) &= \text{radial distribution function (RDF)} \\ w &= \text{relative velocity} \\ P(w \,|\, r) &= \text{PDF of relative velocity} \end{aligned}$$

RDF corrects for preferential concentration (dominant effect at low Stokes numbers)

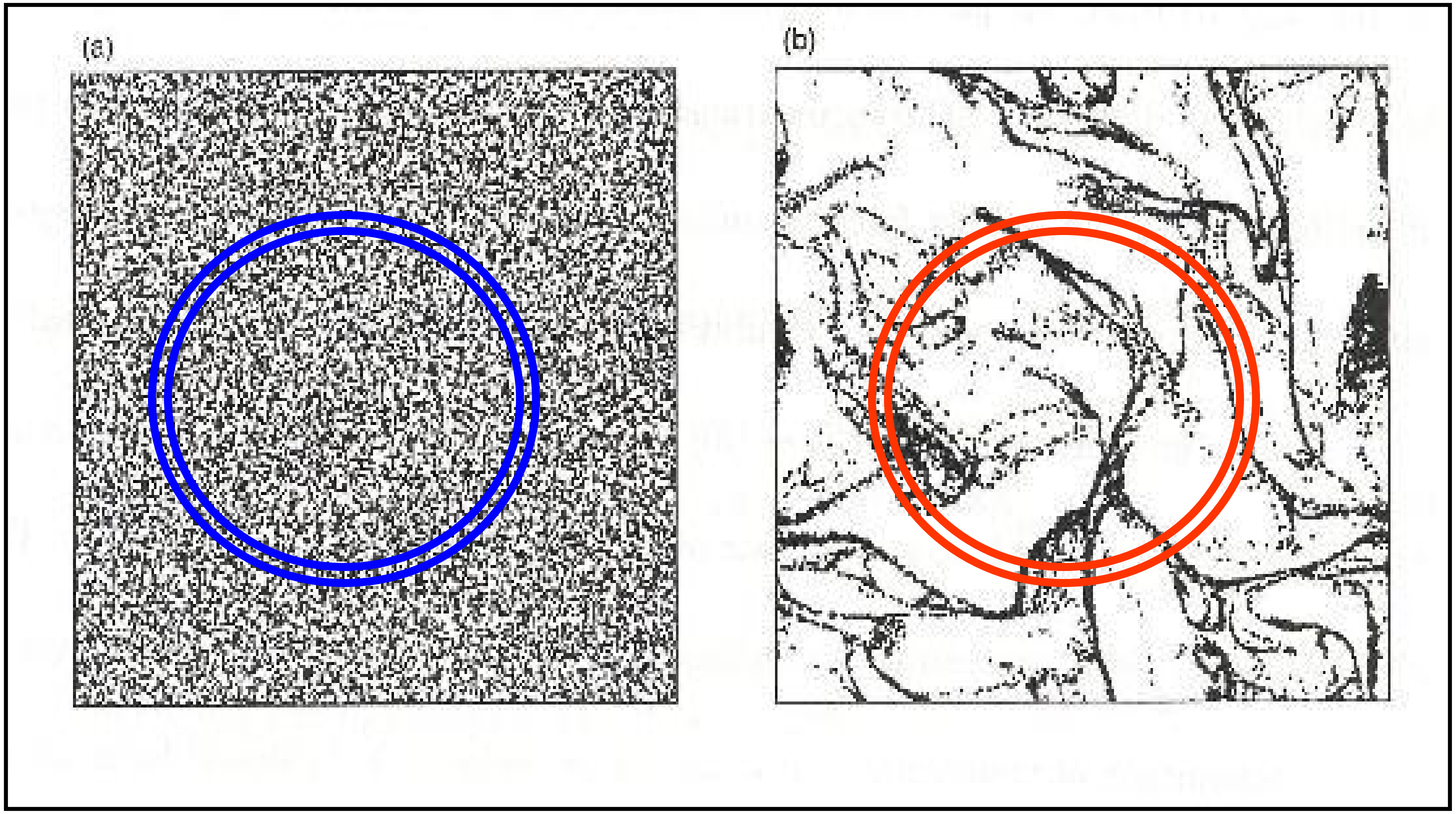
Sundaram & Collins (1997)
Wang, Wexler and Zhou (1998)

RDF

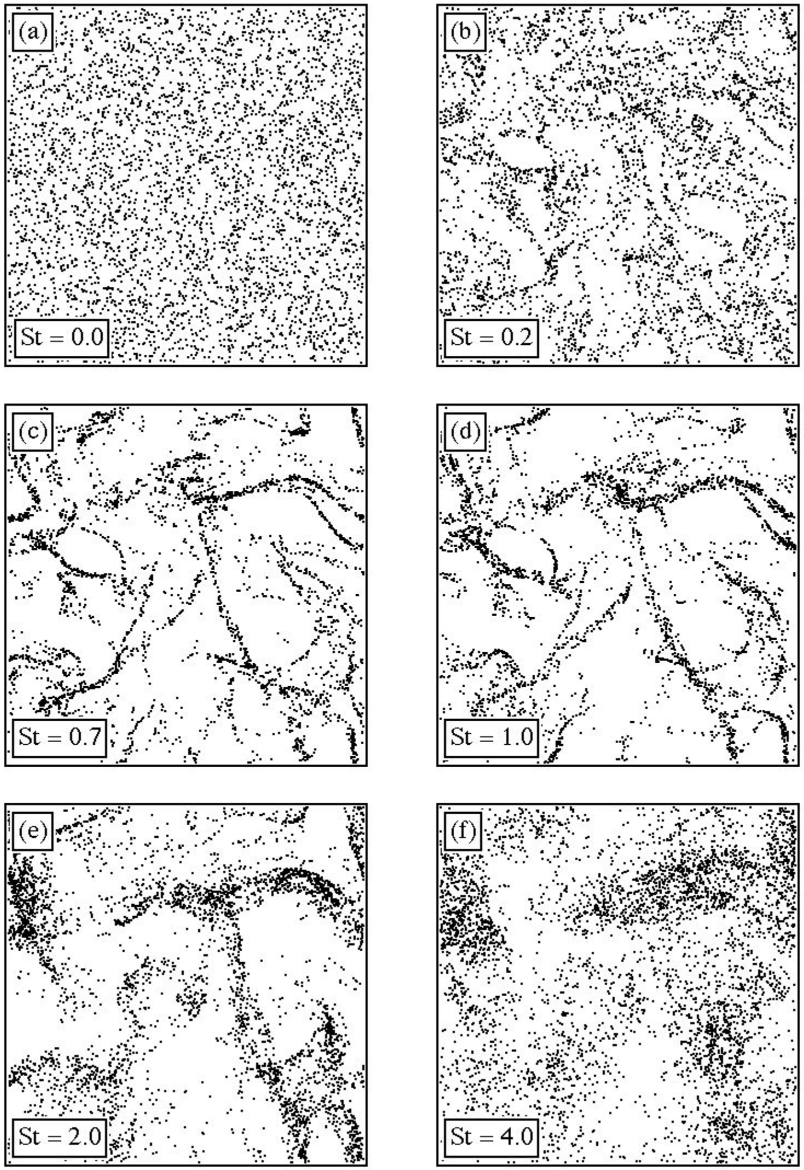
$$g(r) \equiv \frac{\#\ \text{pairs}}{\text{expected}\ \#\ \text{pairs}}$$

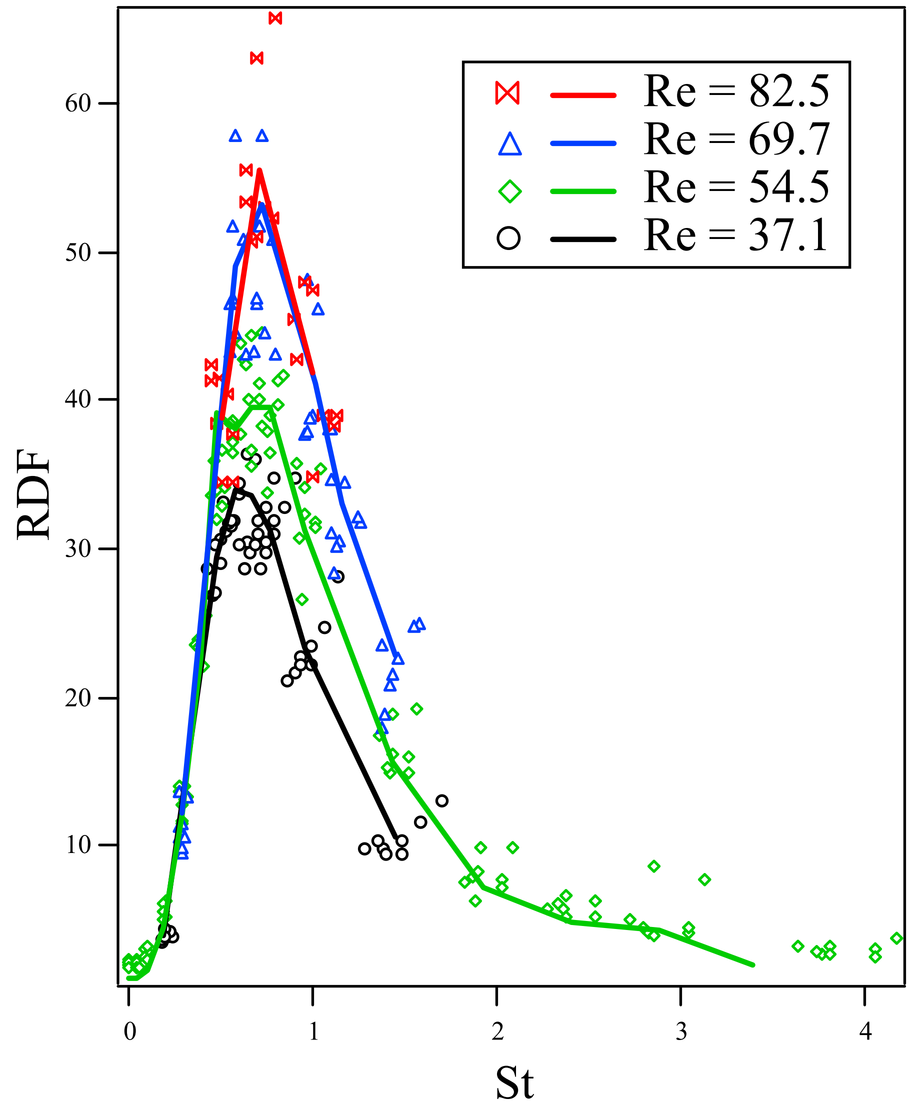
Parametric Dependence

- volume fraction
- Stokes number
- size parameter
- Reynolds number

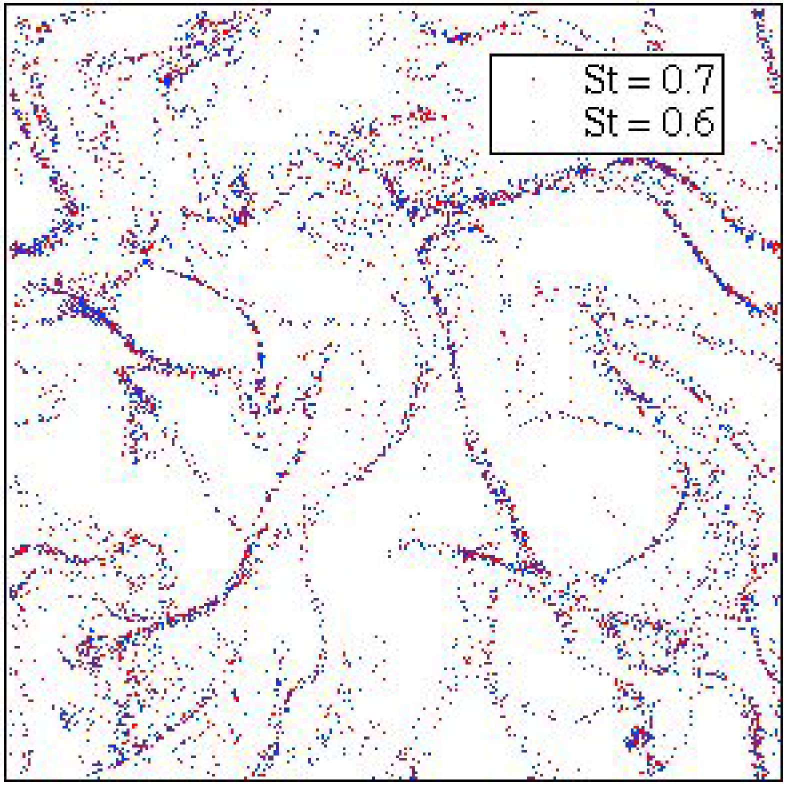


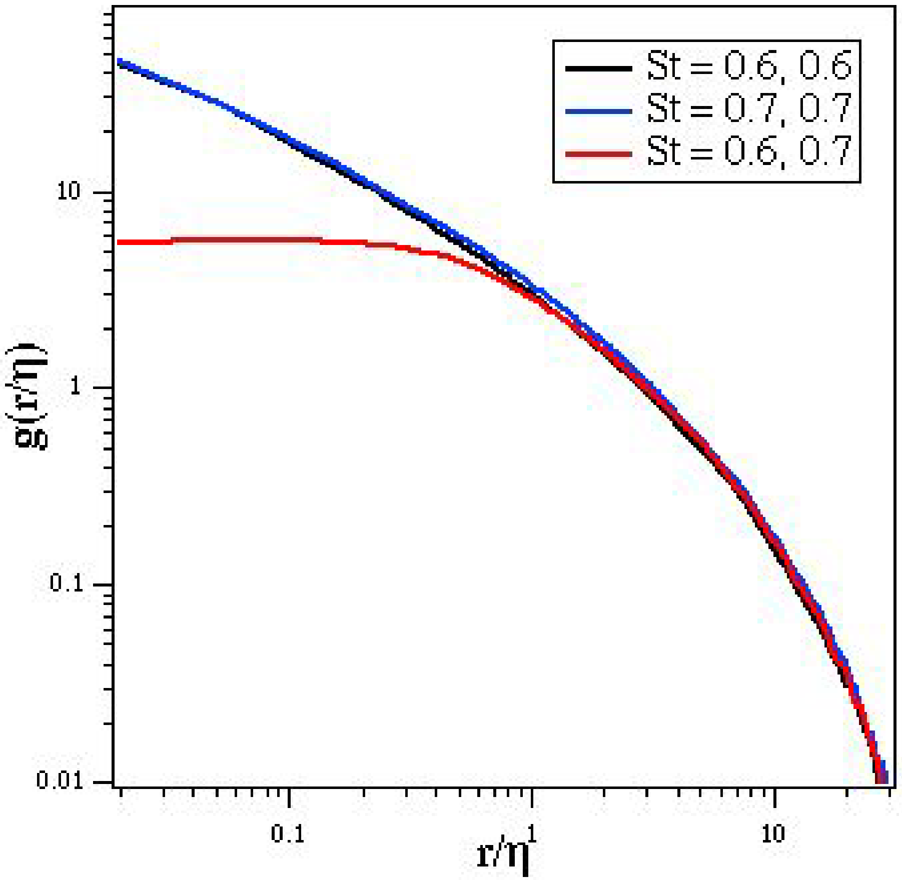
Stokes number dependence





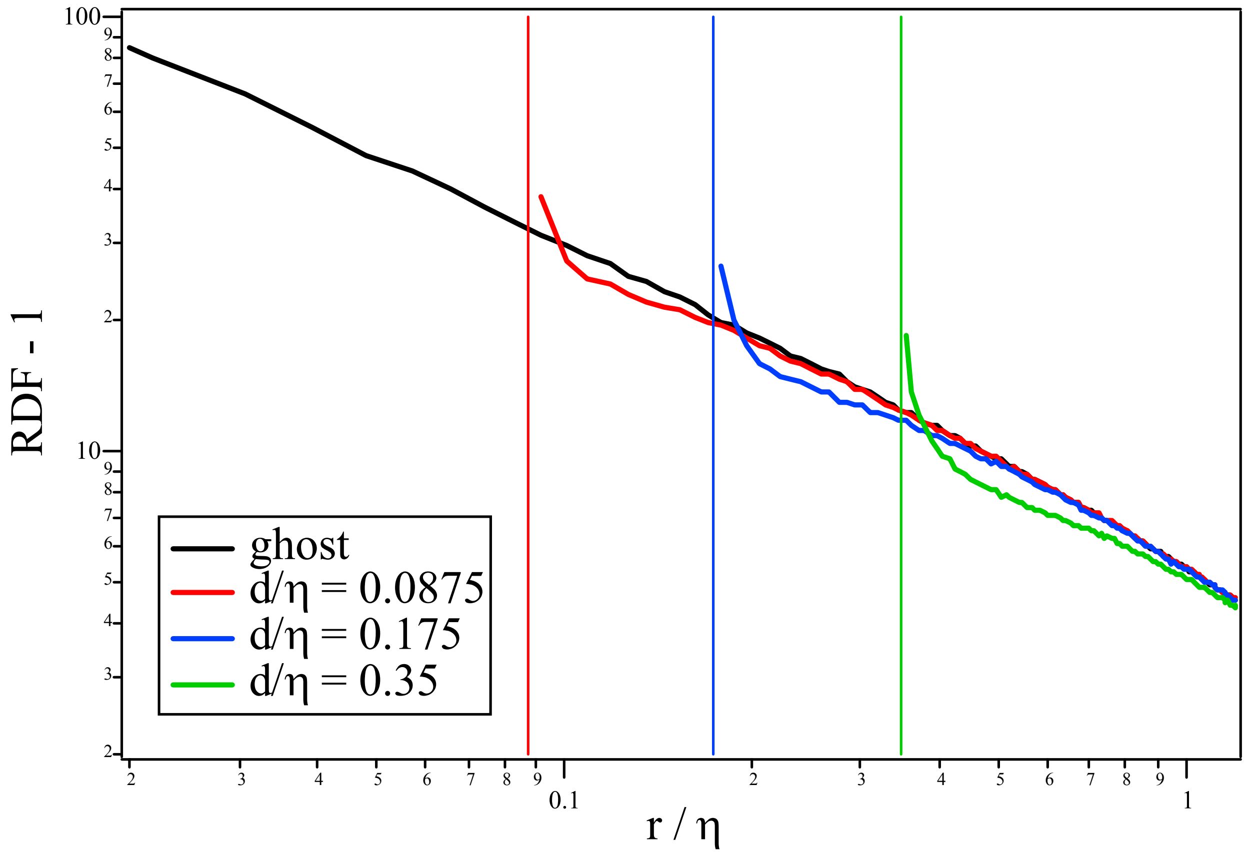
Bi-disperse St dependence



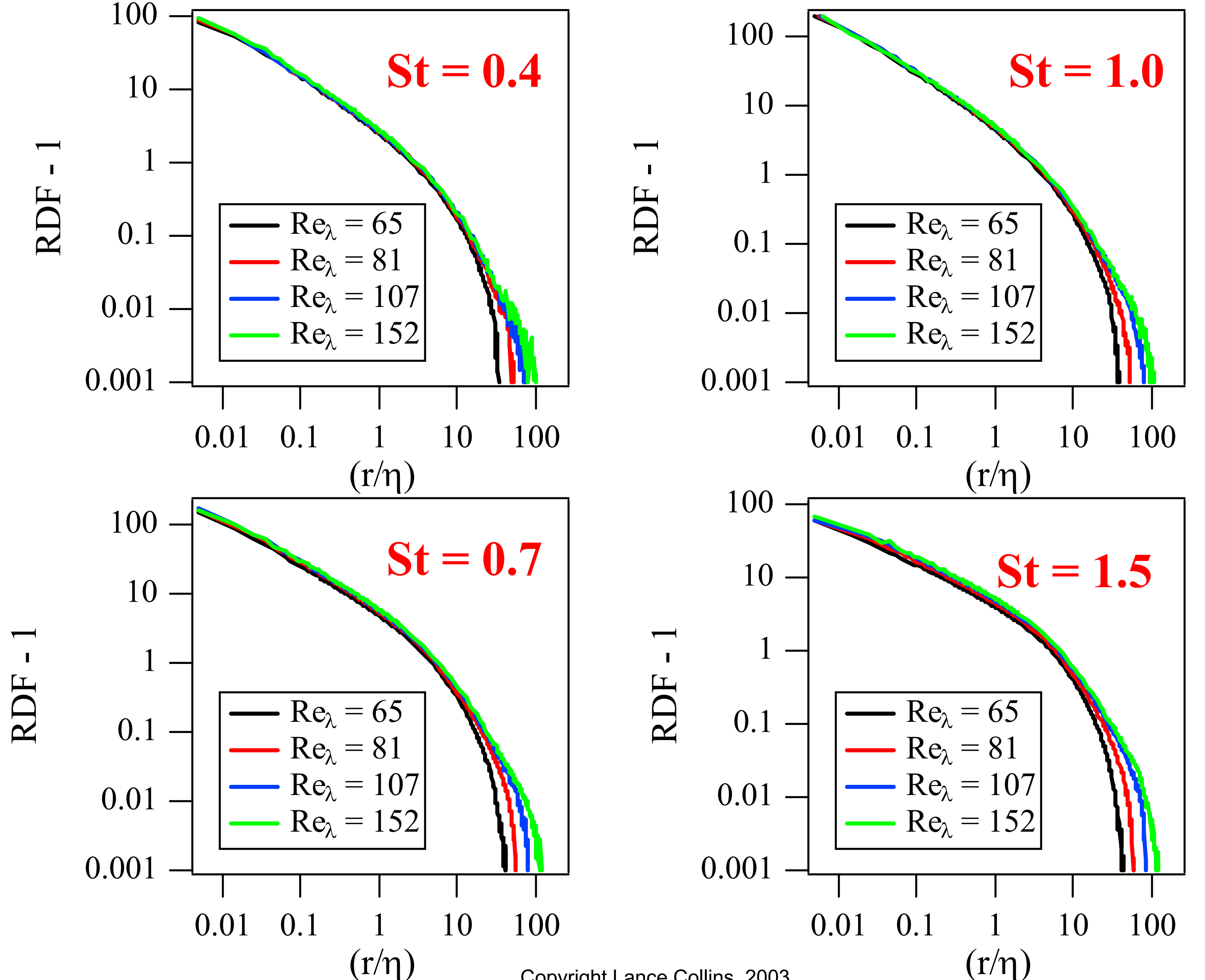


Suppression of off-diagonal collisions broadens the distribution

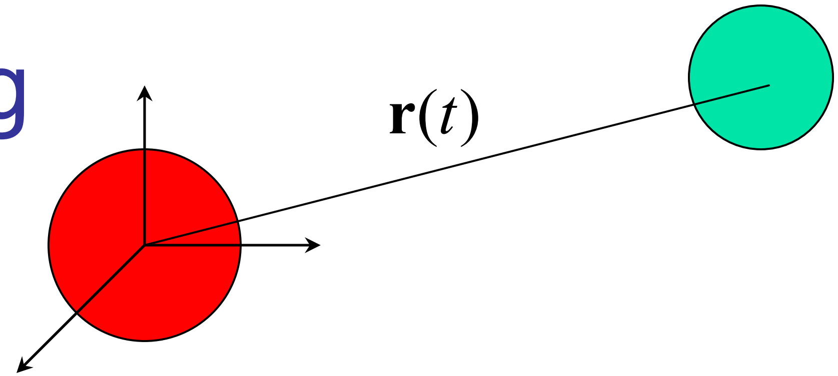
Size parameter



Reynolds Number Dependence



Physics of clustering

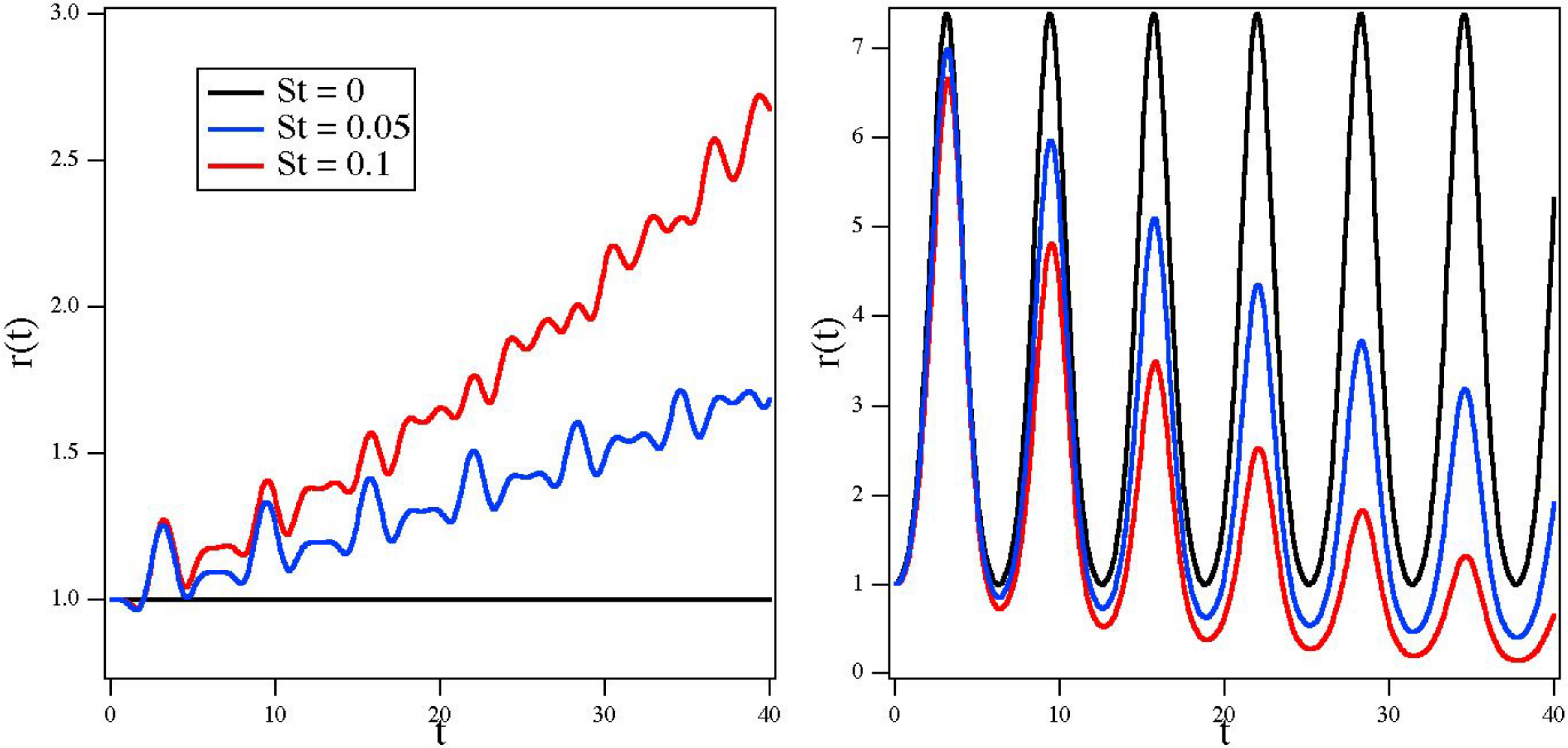


Maxey (1987)

Frame moving with a test particle

Rotation

Strain



Recent Theoretical Developments

- Wang, Wexler & Zhou (2000)

  relative velocity

  clustering effect

- Falkovich, Fouxon and Stepanov (2002)

  clustering effect in clouds

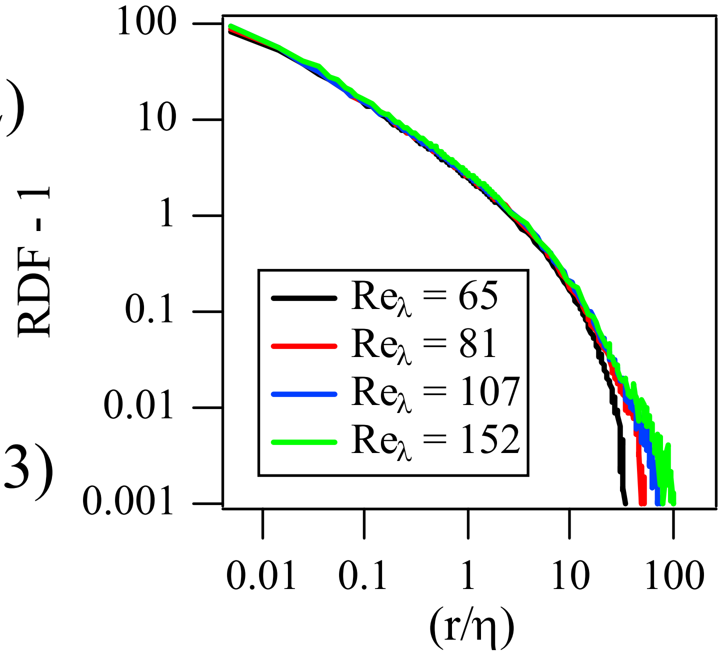
- Zaichik & Alipchenkov (2003)

  relative velocity

  clustering

- Chun, Koch, Ahluwalia & Collins (2003)

  clustering (St << 1)



$$g\left(\frac{r}{\eta}\right) = c_0 \left(\frac{\eta}{r}\right)^{c_1}$$

$$c_0\,(R_\lambda\,,St\,,\not{\Phi})$$

$$c_1\,(R_\lambda\,,St\,,\not{\Phi})$$

Chun et al. (2003) St<<1

$$\frac{\partial g}{\partial t} = -\frac{1}{r^2}\frac{\partial\left(r^2\, A\, r\, g\right)}{\partial r} + \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\, B\, r^2\,\frac{\partial g}{\partial r}\right]$$

nonlocal diffusion

$$A = \frac{St}{3\,\tau_\eta}\left(\left\langle S^2\right\rangle_p - \left\langle R^2\right\rangle_p\right)$$

$$\frac{\Delta\left\langle S^2\right\rangle_p}{St} = \left[\frac{\sigma_\varepsilon^2}{\varepsilon^2}T_{\varepsilon\varepsilon} - \frac{\rho_{\varepsilon\varsigma}\sigma_\varepsilon\,\sigma_\varsigma}{\varepsilon^2}T_{\varepsilon\varsigma}\right], \quad \frac{\Delta\left\langle R^2\right\rangle_p}{St} = \left[\frac{\rho_{\varepsilon\varsigma}\sigma_\varepsilon\,\sigma_\varsigma}{\varepsilon^2}T_{\varsigma\varepsilon} - \frac{\sigma_\varsigma^2}{\varepsilon^2}T_{\varsigma\varsigma}\right]$$

Steady State

$$g(r) = c_0\left(\frac{\eta}{r}\right)^{c_1}$$

$$c_1 = A / B = 6.6\, St^2$$

$$c_1 = 3.6\, St\left(\left\langle S^2\right\rangle_p - \left\langle R^2\right\rangle_p\right)$$

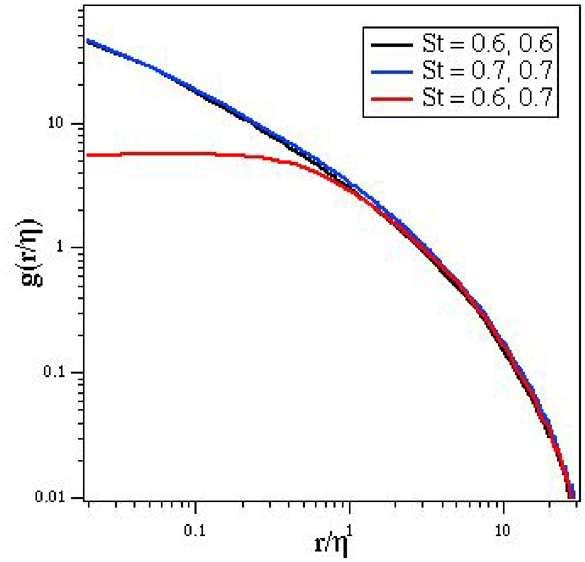
St	DNS	Stoch	Theory
0.05	0.016	0.016	0.017
0.1	0.08	0.07	0.06
0.15	0.15	0.14	0.14
0.2	0.19	0.18	0.17

Chun et al. (2003) Bidisperse

- Fluid accelerations give rise to relative diffusion

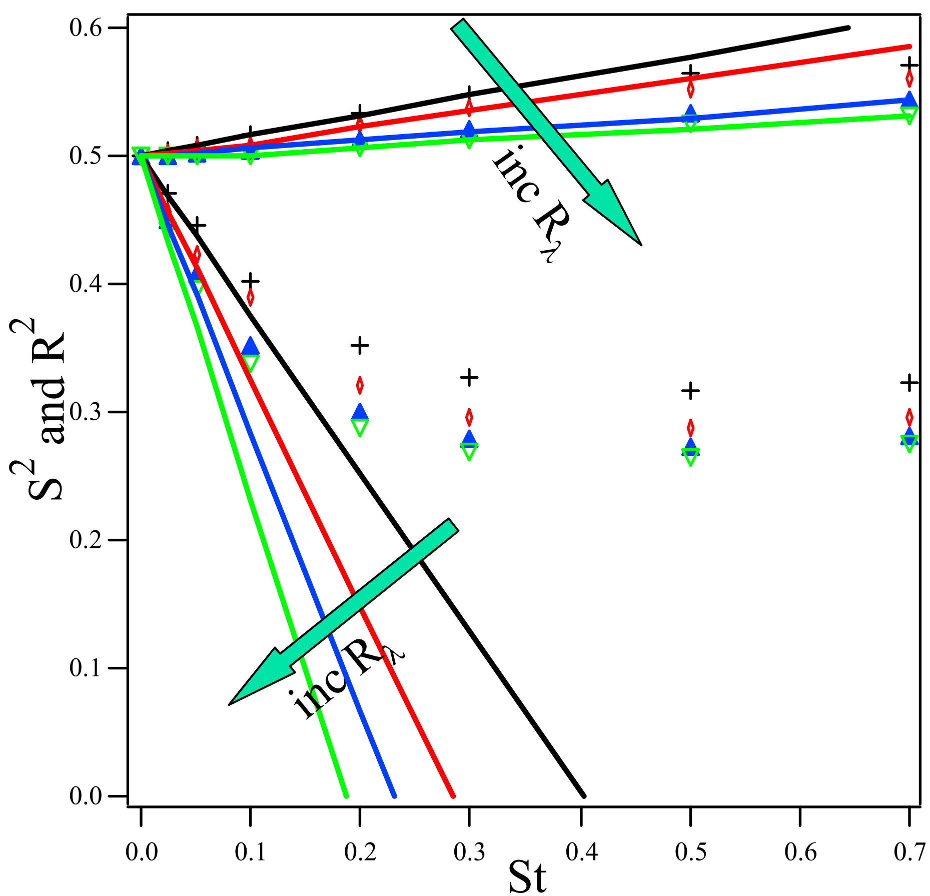
$$g_{AB}(r) = c_0 \left[\frac{\eta^2}{r^2 + r_c^2} \right]^{c_1/2}$$

$$r_c = B' \left| St_A - St_B \right| \eta$$



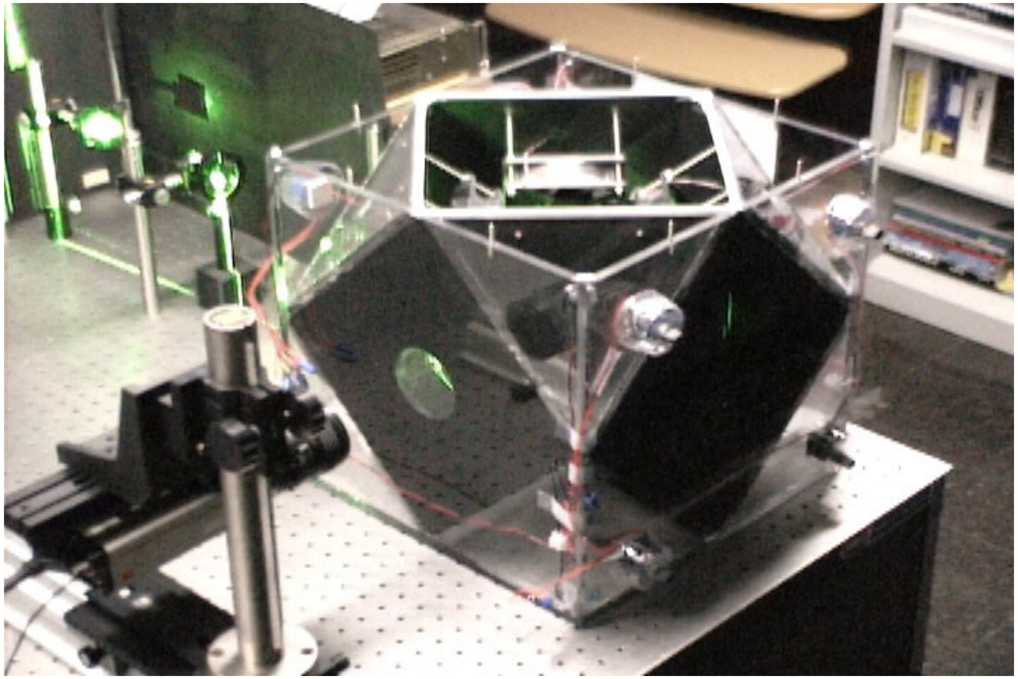
Reynolds Number Dependence

$$c_1 = 3.6\, St \left(\left\langle S^2 \right\rangle_p - \left\langle R^2 \right\rangle_p \right)$$

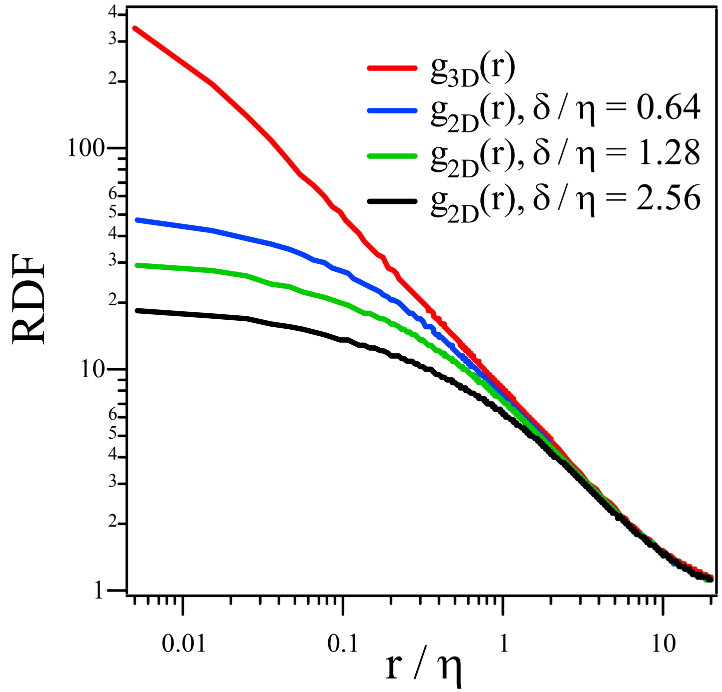


Experimental 3D Particle Imaging

Professor Hui Meng



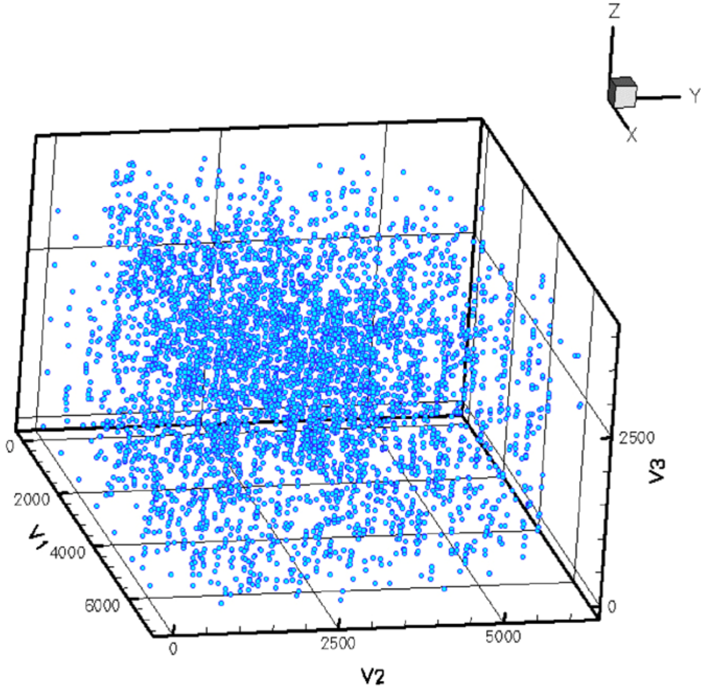
Why 3D?

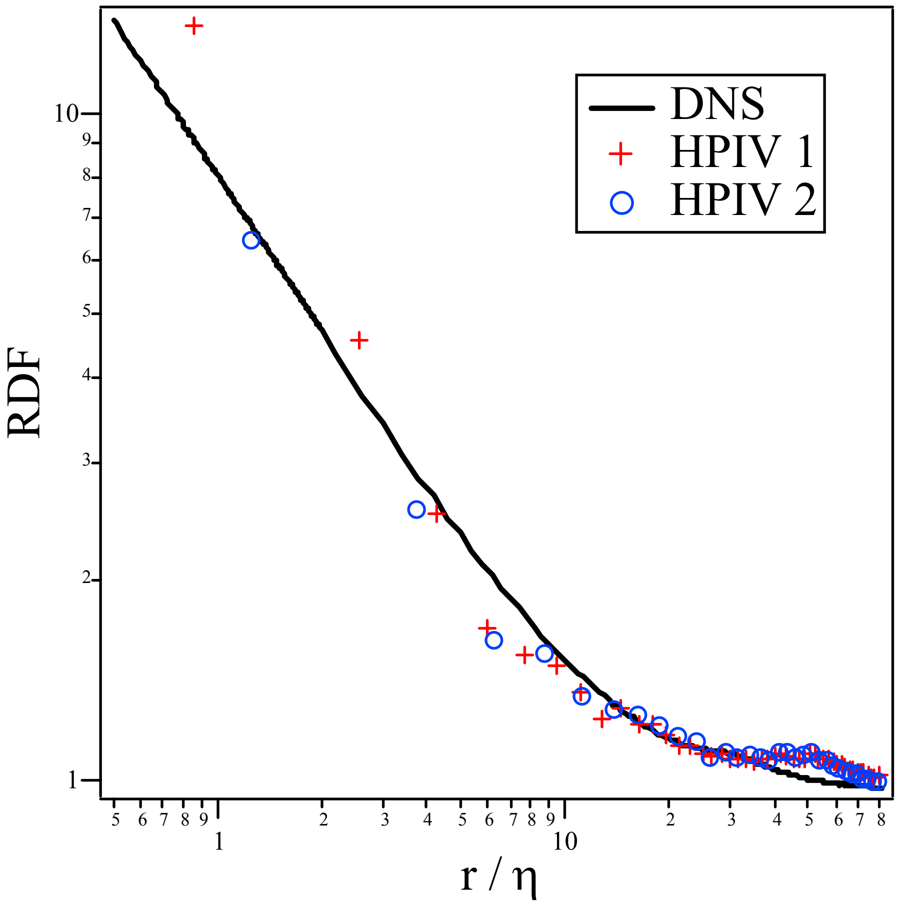


- Cover a Broader Range of R_λ
- Validate DNS and Theory

Holtzer & Collins (2002)

Preliminary Results





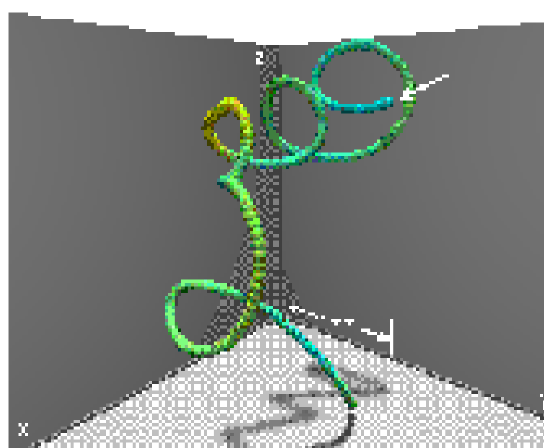
Particle Tracking

Eberhard Bodenschatz and Zellman Warhaft

Wind Tunnel
(active grid)

QuickTime™ and a YUV420 codec decompressor are needed to see this picture.

- Track droplets
  - Multiple (4) cameras
  - High speed (above 50,000 fps)
  - Integral time and length scales
- Measure accelerations
  - Compare with DNS
  - Test theoretical predictions



Droplets
10 - 50 microns

Summary

- **Particle clustering in turbulent flows**
  - Increases collision frequency 1-2 orders of magnitude
  - Strongly favors like collisions; broadens particle size distribution
- **Theoretical predictions for RDF**
  - Stokes number dependence
  - Size parameter
  - Reynolds number dependence remains in dispute (key for cloud physics)
- **Experiments**
  - Validate DNS and theory
  - Increase the range of Reynolds numbers
- **Enabling Technologies**
  - 3D imaging essential
  - Holographic imaging (RDF at an instant)
  - High-Speed Stereoscopic Tracking (Lagrangian statistics)

DNS has continuously guided theoretical and experimental work

Acknowledgments

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- Prof. R. Shaw (Mich. Tech)
- Prof. M. Loewenberg (Yale)

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- W. Reade (Kimberly Clark)
- A. Keswani (Goldman Sachs)
- A. Ahluwalia (Epic Sys.)
- S. Rani

Undergraduate Students
- Carolyn Nestleroth
- Melissa Feeney
- Anthony Fick

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PHY-0216406

Future Work

- High-resolution DNS (JC.001)
  - Effect of shear flow
  - Hydrodynamic interactions
- Extend theory to coalescing system
- Experimental measurements
  - HPIV at an instant
  - Lagrangian statistics