DIRECT NUMERICAL SIMULATION OF LIQUID-SOLID FLOW

http://www.aem.umn.edu/Solid-Liquid_Flows

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Fluid Mechanics & CFD

D.D. Joseph
R. Glowinski
H. Hu
P. Singh
T.W. Pan
P.Y. Huang
N. Patankar
H.G. Choi
T. Hesla
M.Y. Zhu

Computer Scientists

Y. Saad
A. Sameh
G. Golub
A. Wathen
V. Sarin
M. Knepley

Industrial partners: Schlumberger, Dowell-Schlumberger, Shell-Houston, Stimlab, Intevep S.A.

The marriage of CFD & CS is very desirable for the future of DNS but it is difficult to achieve.

METHODS FOR STUDYING MULTIPHASE PROCESSES

- **Experiments**
- **Analysis (mathematical models)**
- **Numerical simulation (computers)**

Experiments and analysis are traditional methods used for hundreds of years without the help of big computers. They are the basis of science and engineering.

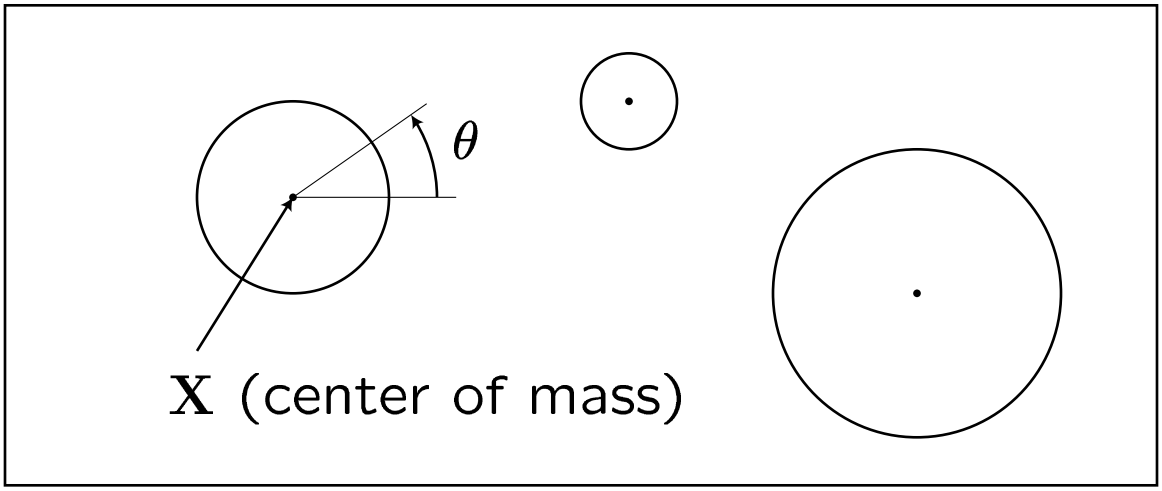
We understand well the uses of traditional methods. Traditional methods are as useful today and into the future as they ever were.

Computers are always being used in new ways. We don’t yet understand what the future of computations may hold. The horizons are not in view; this is a good environment for visionary research.

DIRECT NUMERICAL SIMULATION (DNS)

Solves the dynamic problem of the motion of particles in a fluid exactly (in principle). The particles are moved by Newton’s laws under the action of hydrodynamic forces computed from the numerical solution of the fluid equations (Navier-Stokes equations for water, etc.)

GOVERNING EQUATIONS



Fluid:

$$\rho_{\mathsf{f}}\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\boldsymbol{\nabla}\mathbf{u}\right) = \rho_{\mathsf{f}}\,\mathbf{g} - \boldsymbol{\nabla} p + \mu\nabla^2\mathbf{u},$$

$$\boldsymbol{\nabla}\cdot\mathbf{u} = 0$$

Particles:

$$M\frac{d\mathbf{U}}{dt} = M\mathbf{g} + \mathbf{F}[\mathbf{u}], \qquad I\frac{d\omega}{dt} = T[\mathbf{u}],$$

$$\frac{d\mathbf{X}}{dt} = \mathbf{U}, \qquad \frac{d\theta}{dt} = \omega$$

No Slip Condition:

$$\mathbf{u} = \mathbf{U} + \omega \times \mathbf{r} \qquad \text{on particle boundaries}$$

The fluid and particle equations of motion can be combined into a **single weak equation of motion**, which governs the evolution of the **total momentum** of the system—fluid plus particle; the force $\mathbf{F}[\mathbf{u}]$ and torque $T[\mathbf{u}]$ cancel out and do not need to be computed.

Find $\mathbf{u}$, p, $\mathbf{U}$, and ω satisfying

$$\int_{\text{fluid}} \rho_{\text{f}} \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \boldsymbol{\nabla} \mathbf{u} - \mathbf{g} \right) \cdot \mathbf{v} \, d\mathbf{x}$$
$$- \int_{\text{fluid}} p \boldsymbol{\nabla} \cdot \mathbf{v} \, d\mathbf{x} + \int_{\text{fluid}} 2\mu \mathbf{D}[\mathbf{u}] : \mathbf{D}[\mathbf{v}] \, d\mathbf{x}$$
$$+ M \left(\frac{d\mathbf{U}}{dt} - \mathbf{g} \right) \cdot \mathbf{V} + I \frac{d\omega}{dt} \xi = 0$$
$$\text{for all } \mathbf{v}, \mathbf{V}, \xi,$$

$$\int_{\text{fluid}} q \boldsymbol{\nabla} \cdot \mathbf{u} \, d\mathbf{x} = 0 \qquad \text{for all } q.$$

$\mathbf{u}$ and $\mathbf{v}$ are *both* required to satisfy the no-slip condition on the particle boundary:

$$\mathbf{u} = \mathbf{U} + \omega \times \mathbf{r} \qquad \mathbf{v} = \mathbf{V} + \xi \times \mathbf{r}$$

Since **DNS** does not use approximations it can be the **STANDARD OF EXCELLENCE** for approximate methods like

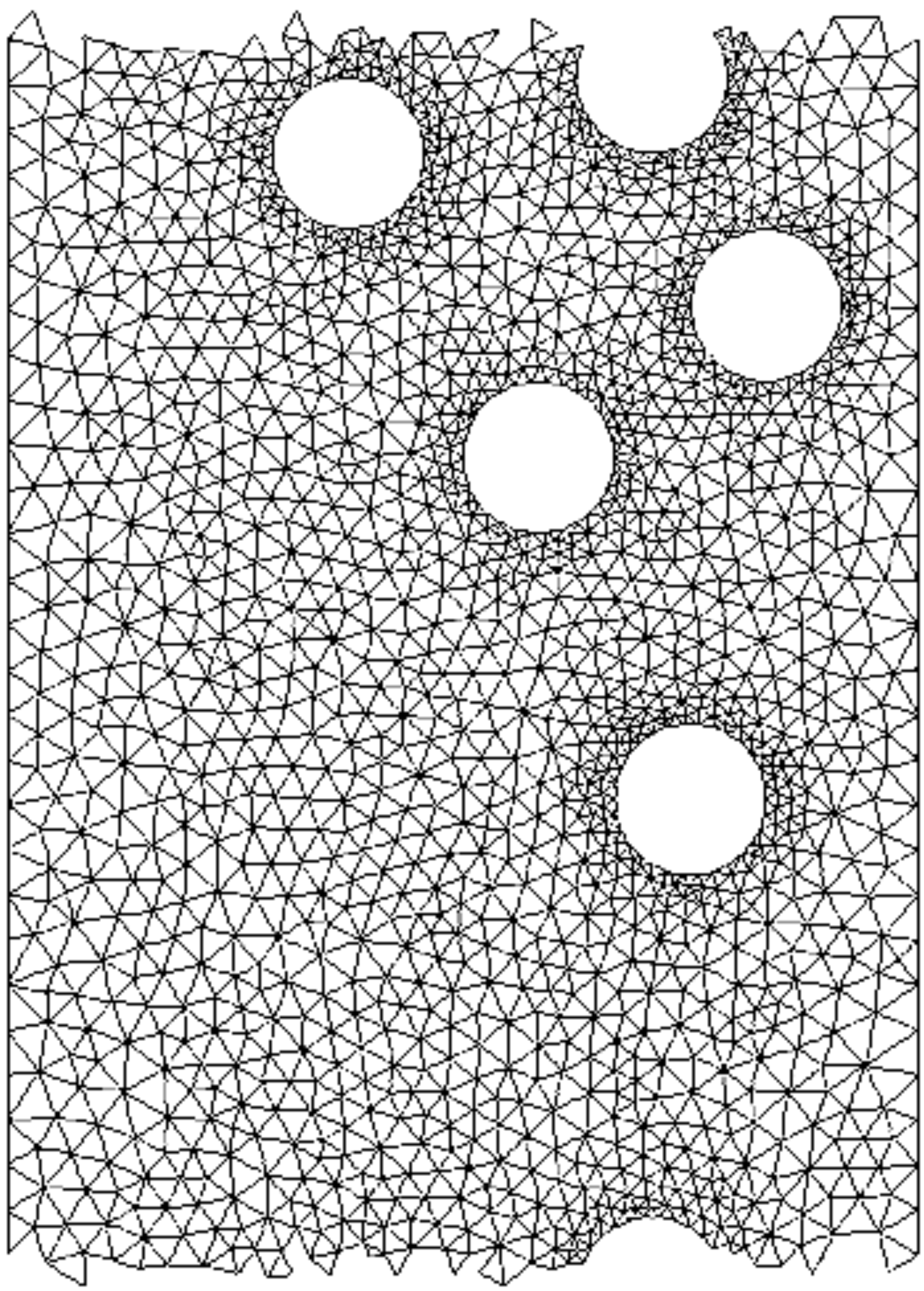
{ DNS for turbulence
LNS Lagrangian numerical simulation
LB Lattice Boltzmann
MIXTURE THEORY

in which the forces on particles are modeled rather than computed.

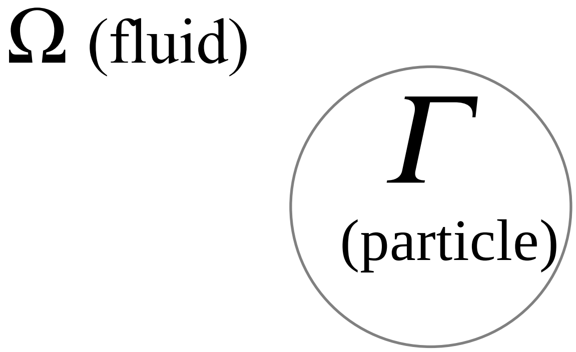
Approximate theories should be validated against DNS.

NUMERICAL PACKAGES FOR MOVING PARTICLES IN DIRECT SIMULATION

(1) Package based on moving unstructured grids is presently a monopoly; it is the only package which can move particles in a viscoelastic fluid in DNS.



(2) Package based on fixed grids in which particles are represented by a field of Lagrange multipliers $\lambda(\mathbf{x},t)$



$$\rho \frac{d\mathbf{u}}{dt} = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{f}$$

div $\mathbf{u} = 0$

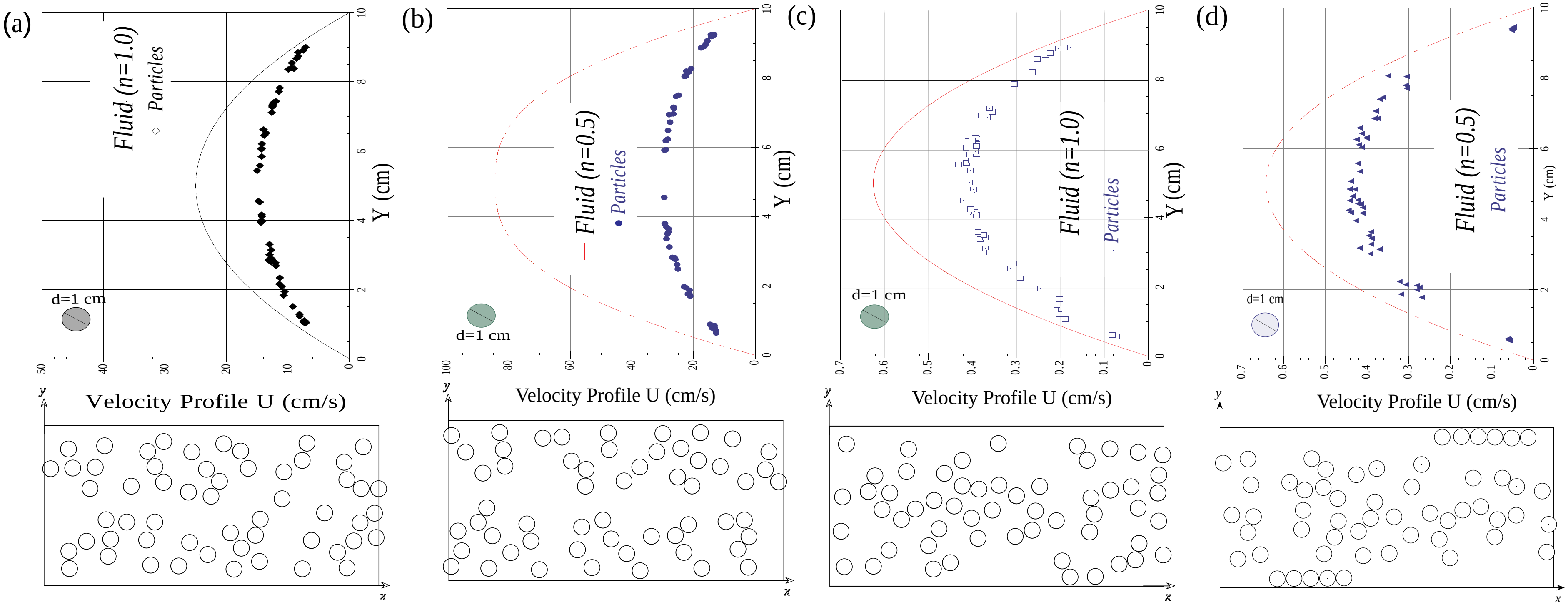
$\mathbf{f} = 0$ in fluid Ω

$\mathbf{f} = \Delta^2 \lambda - \lambda$ in Γ together with constraint

$\mathbf{u} = \mathbf{U} + \omega \times \mathbf{r}$ in Γ

$\lambda(\mathbf{x},t)$ guarantees that the fluid moves rigidly in Γ

APPLICATIONS
OF
DNS

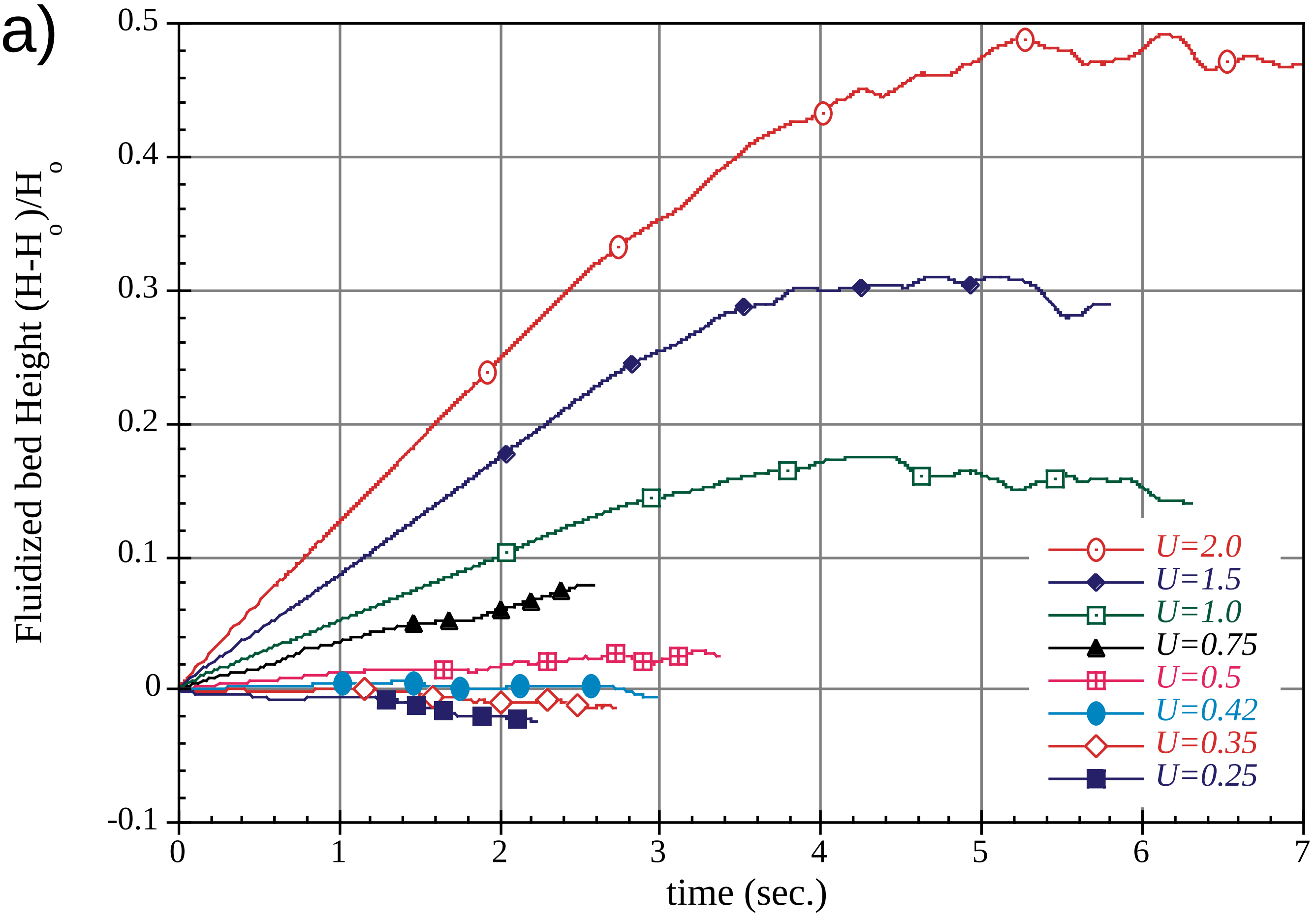


Migration of neutrally bouyant particles in pressure driven flow by DNS.

You can isolate and study effects by switching physics on and off in the simulations that you could not do in experiments. (a) Newtonian, (b) Generalized Newtonian with shear thinning index $n = 0.5$, (c) viscoelastic, (d) viscoelastic with shear thinning.

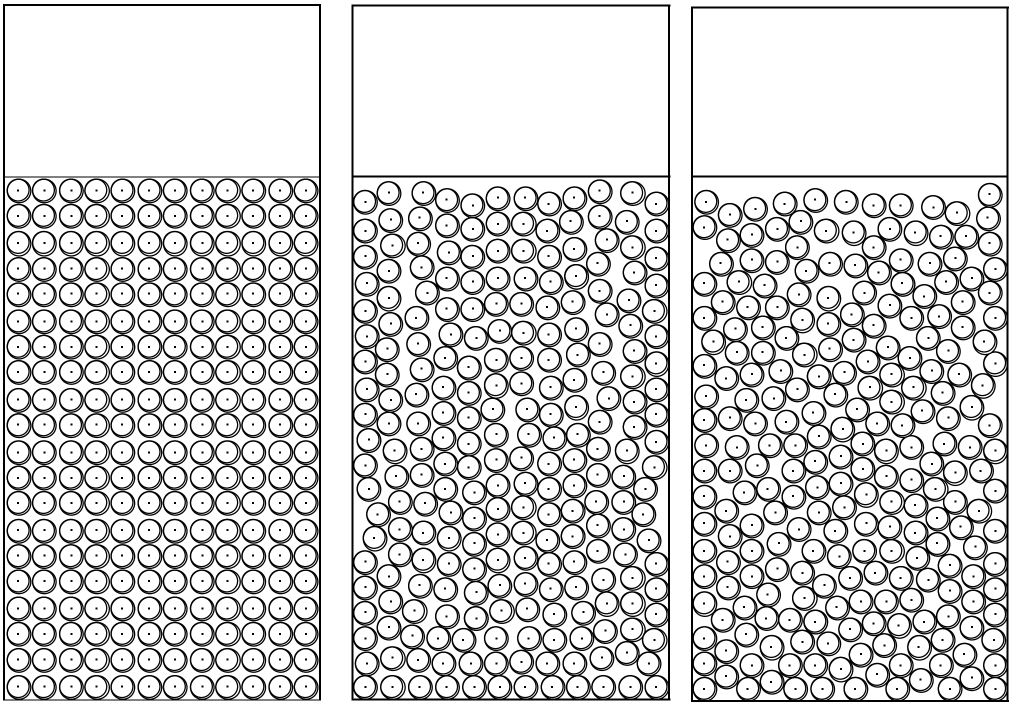
SURROGATE FOR EXPERIMENTS, BED EXPANSION OF A FLUIDIZED BED

(a)



U = 1.0 cm/s

(b)



UNDERSTANDING MICROSTRUCTURE

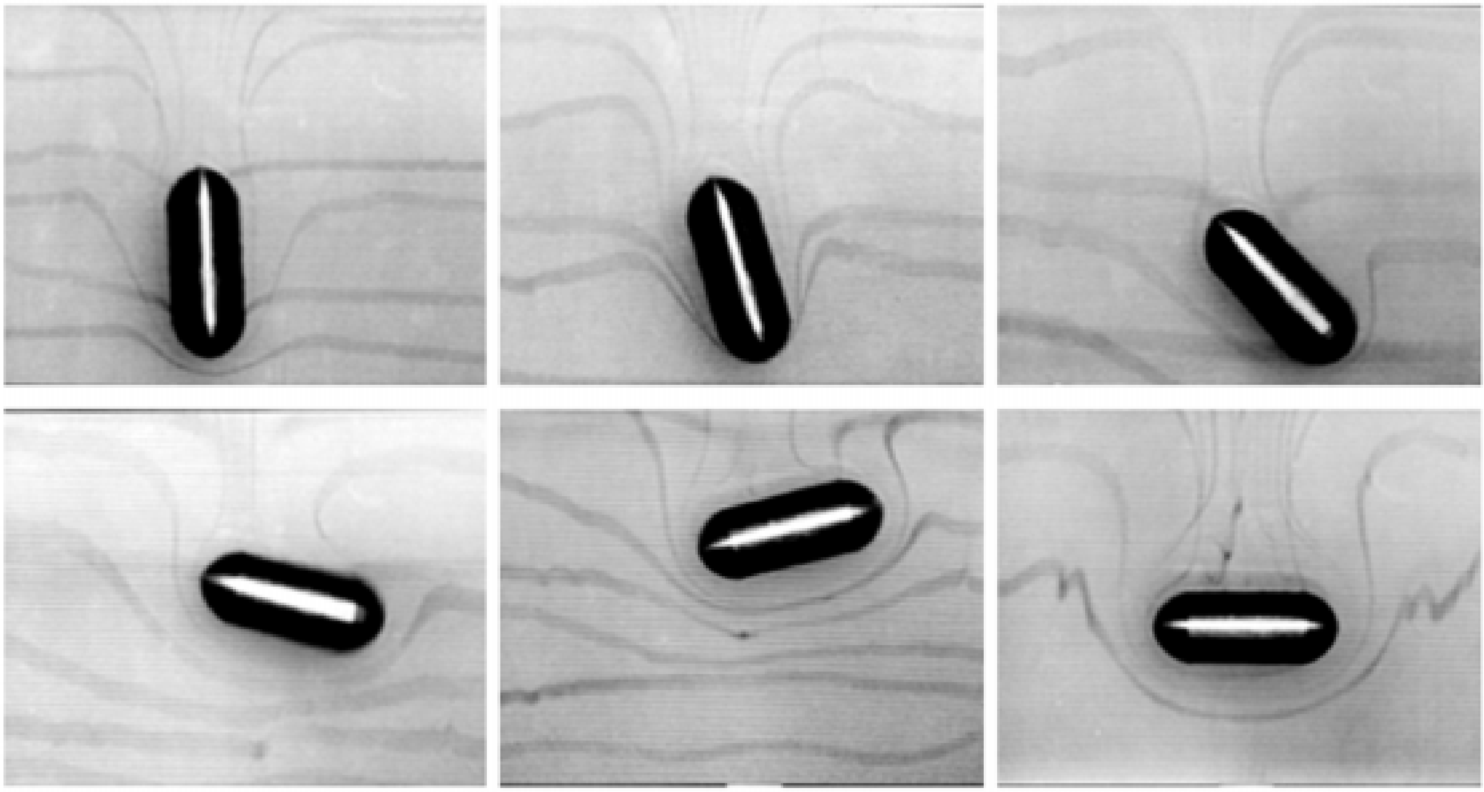
There is a microstructure which is induced by the fluid dynamics of falling bodies and is governed by very simple principles. Long bodies are stable across the stream in Newtonian fluids, but along the stream in non-Newtonian fluids. Spherical particles form arrays across the stream in Newtonian fluids and along the stream in non-Newtonian fluids.

The Mechanisms which determine the microstructure of falling sphereical bodies are wakes and, surprisingly, the turning couples on long bodies, like cylinders or flat plates.

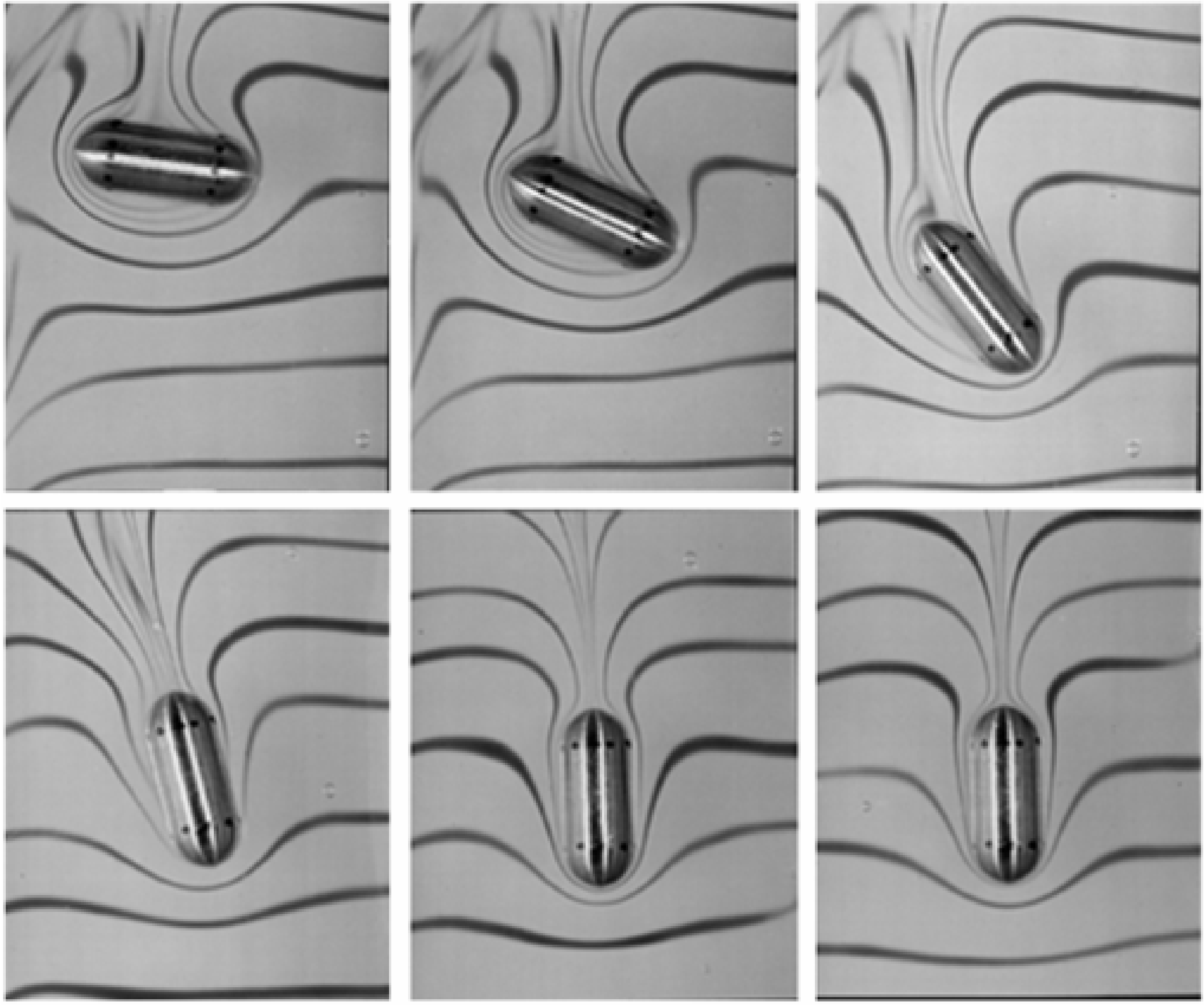
The pressures in a Newtonian fluid are **greatest** near a stagnation point on the body where the **flow is slow.**

There are pressure in a non-Newtonian fluid due to normal stresses, which don’t exist in Newtonian fluids, and these pressures are **greatest** at points on the body where the **flow is fast**.

The flow microstructures which develop in Newtonian and non-Newtonian fluids are maximally different because the underlying pressures which act on the body are greatest at opposite places on the body.



Cylinders falling in a Newtonian fluid turn their long axis perpendicular to the fall. An airplane will stall or a sailing ship will turn its broadside across the wind if not controlled.

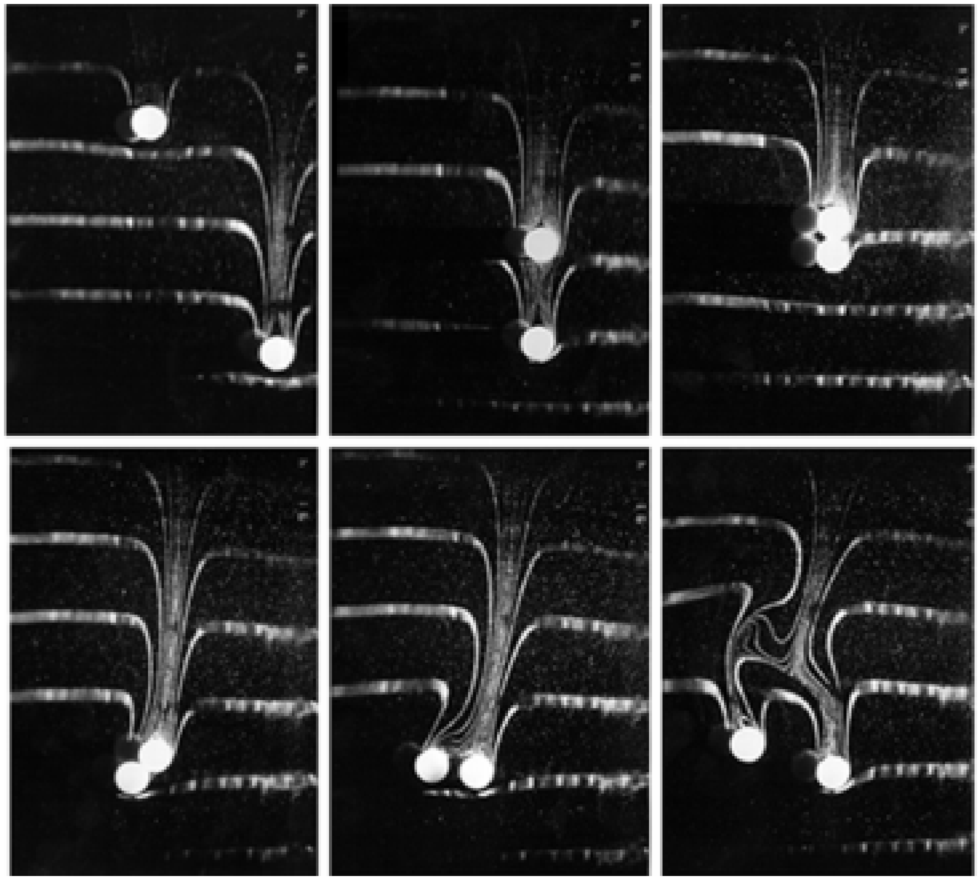


Cylinders falling in a Viscoelastic fluid turn their long axis parallel to the flow, the exact opposite of a Newtonian fluid. An airship in a viscoelastic fluid would not stall and it would not fly.

Spheres in Newtonian Fluids

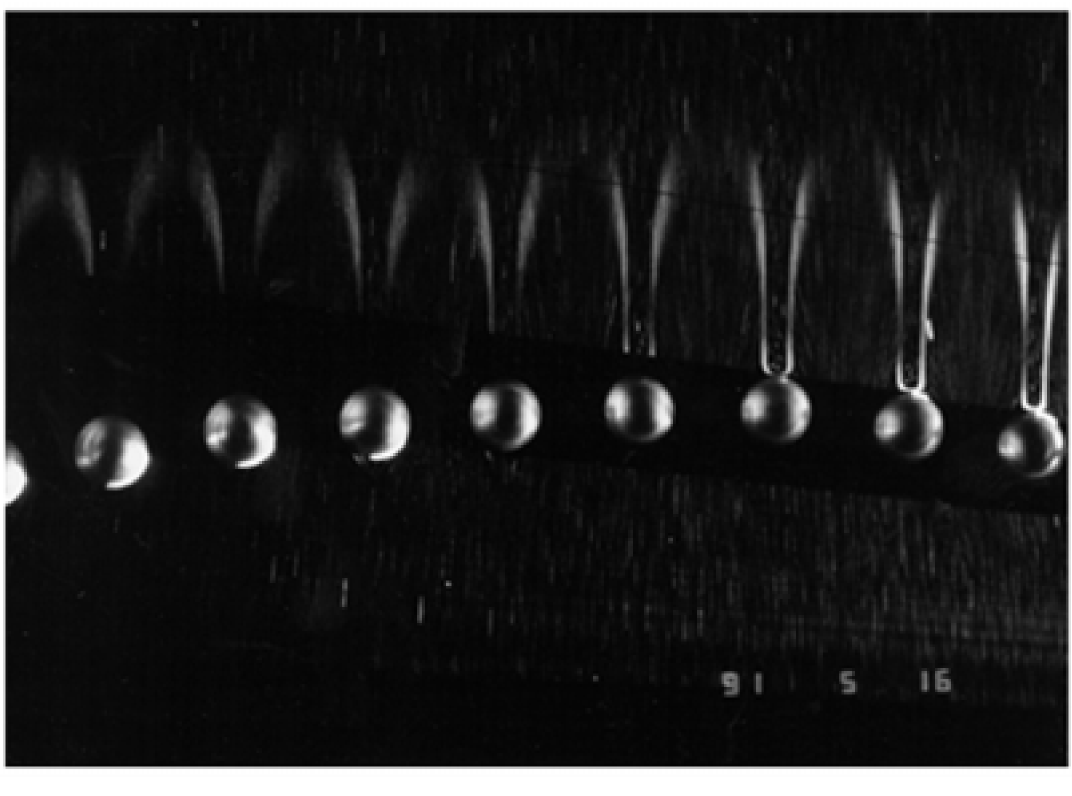
Spheres fluidized in glycerin **draft, kiss and tumble**. They tumble because kissing spheres are a long body which is unstable when its long axis is parallel to the stream.

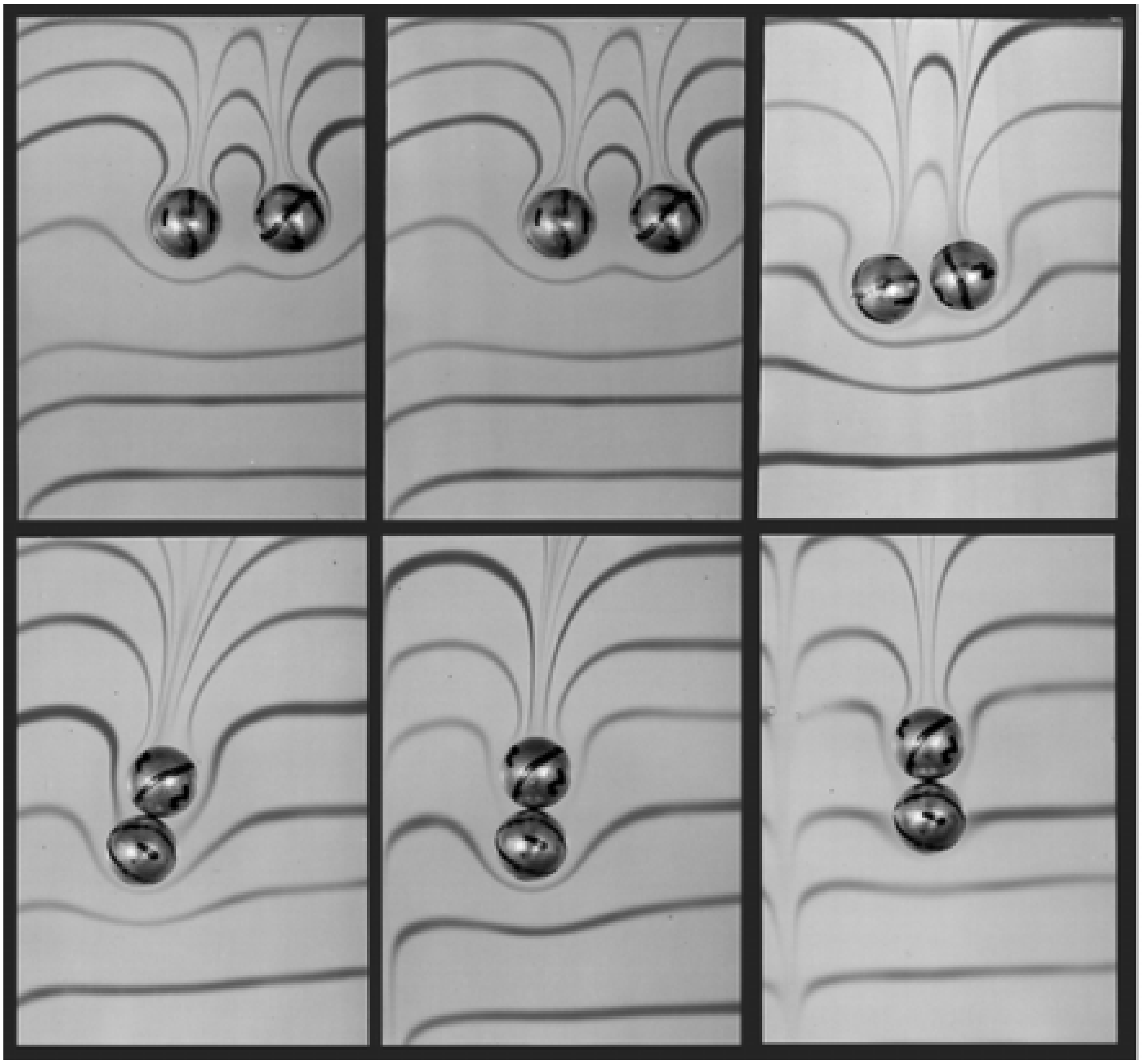
The forces in a Newtonian fluid are dispersive; the tumbling spheres are pushed apart.

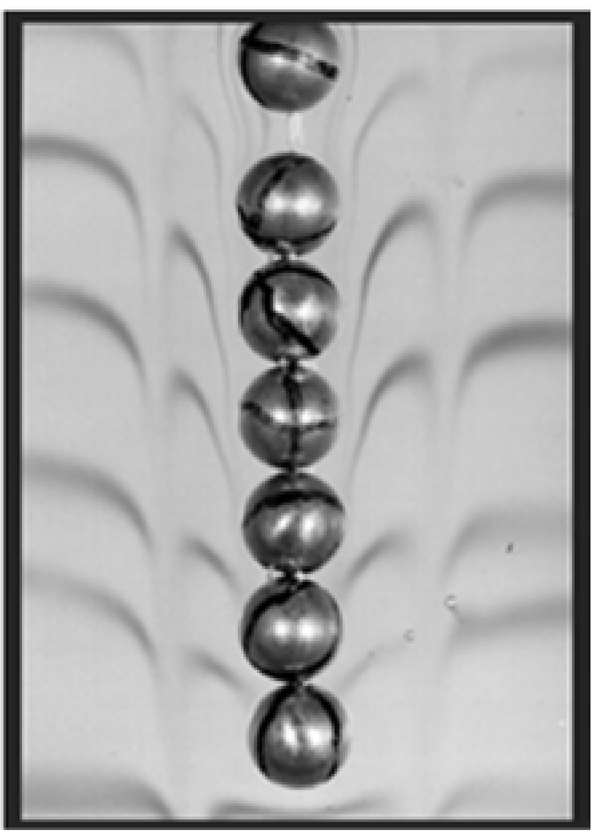


Spherical Particles Form Arrays In Newtonian Fluids

Fourteen spheres line up in a stable array across the stream as if they were a long body.



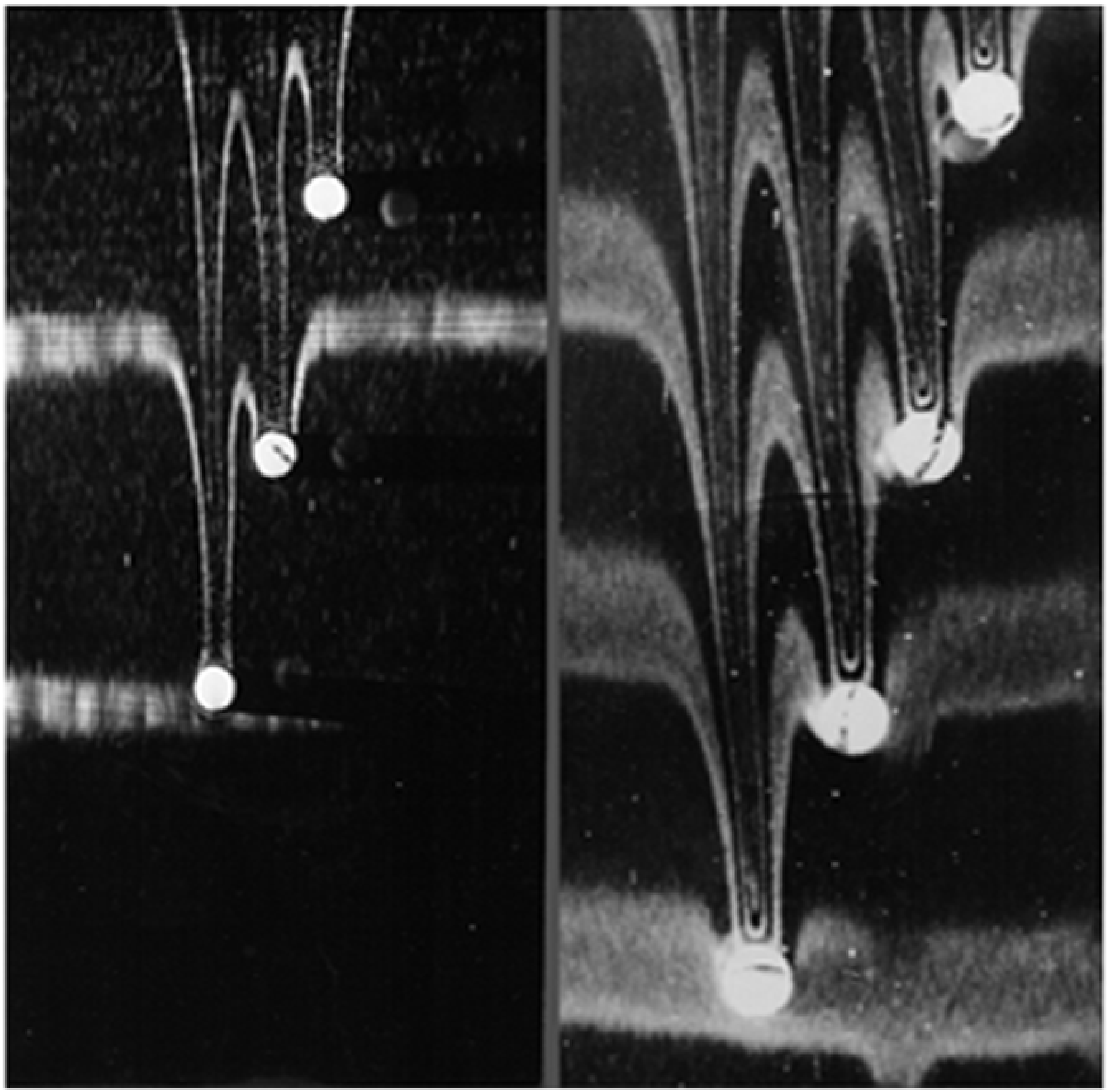




Spheres in Non-Newtonian Fluids

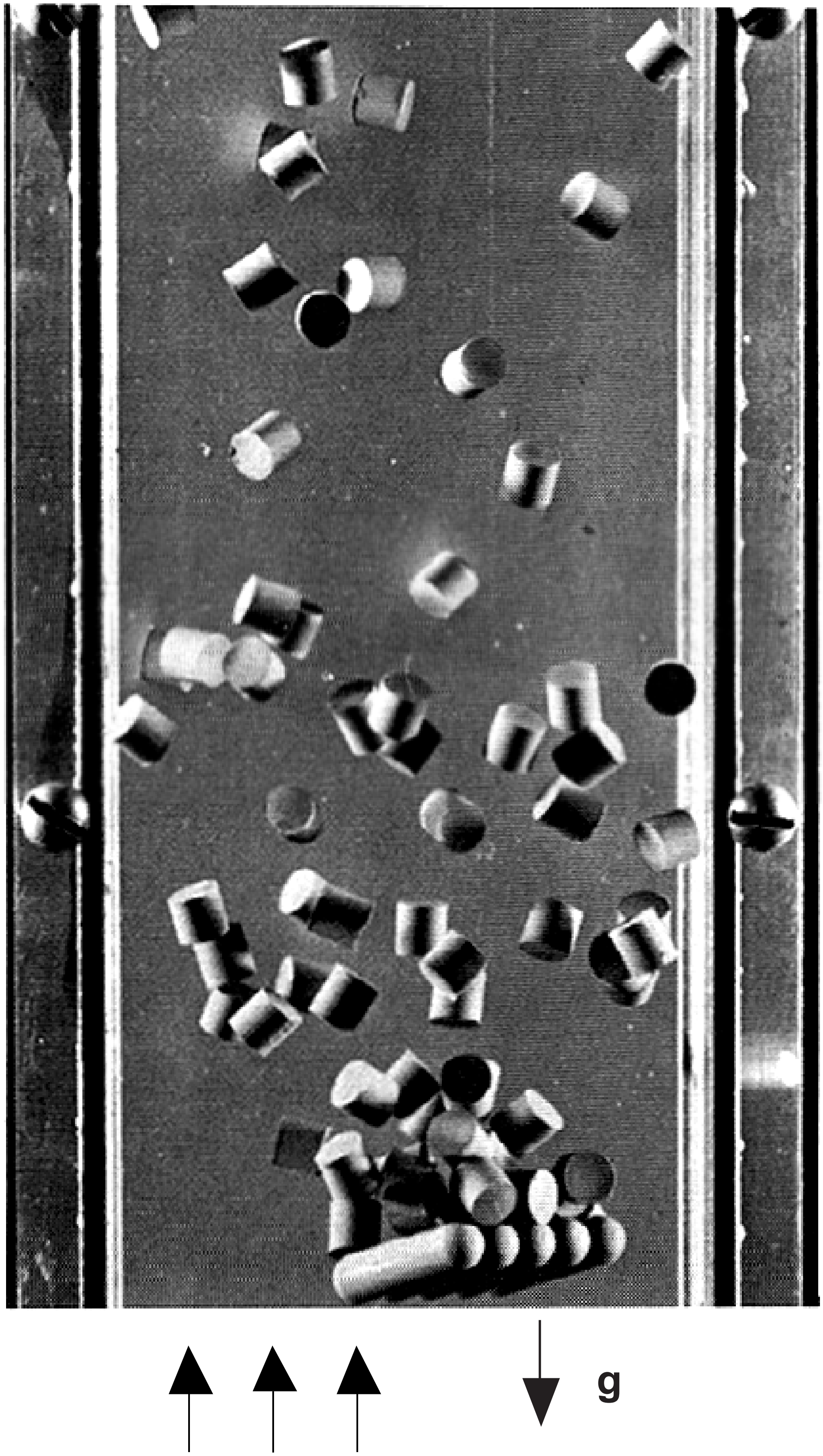
(Above) Spheres falling in 2% polyox in 98% water **draft, kiss and chain**. They chain because the **forces in a viscoelastic fluid are aggregative**. Chained spheres are a long body which is stable with its long axis vertical. The chained spheres turn just like the solid cylinder. Reversing time, we see that chaining, kissing and drafting are like drafting, kissing and tumbling.

(Left) Spheres are falling with their long axis vertical and along the stream, stable and permanently chained.



Spherical Particles in Newtonian Fluids Form Like Birds in Flight

When 22<**Re**<43, the spheres do not draft, kiss and tumble. Three and four of them form a permanent nested wake structure in which each successive sphere is nested in the wake of the one before and it rotates in a shear field there. This reminds us of the **formation of birds in flight**.



FLUIDIZED RAFT PERPENDICULAR TO U

A raft was constructed by gluing long cylinders. It turns broadside on and collects particles in its wake, like debris behind a truck.

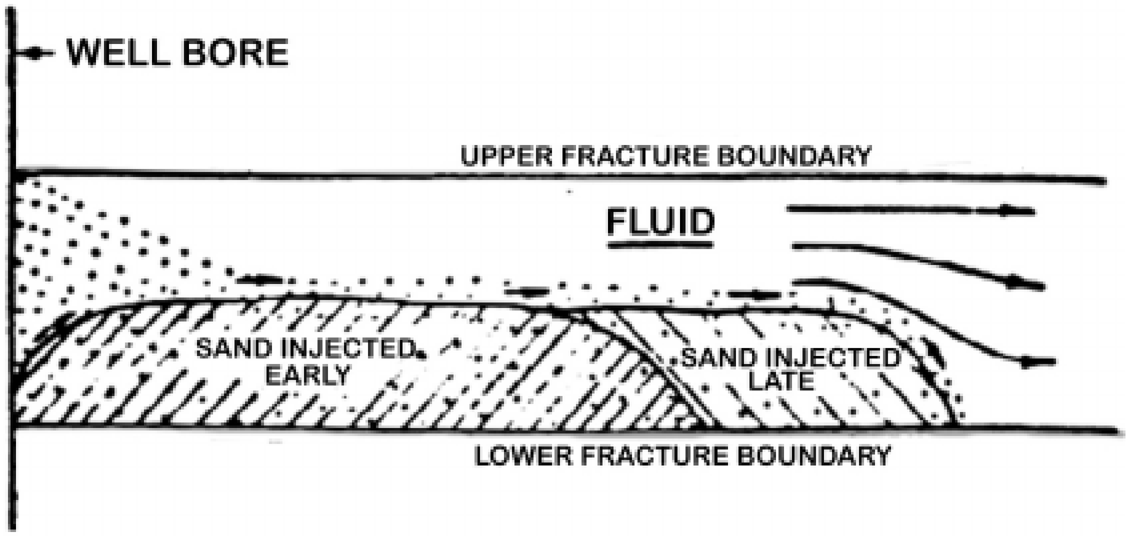
TWO PHASE FLOW MODELS (MIXTURE THEORY, LNS) DO NOT PREDICT:

- Long bodies stable broad side on
- Drafting, Kissing, and Tumbling
- Across the stream arrays of spheres
- Nested wake structure, “Flying Birds”
- Doublets, Triplets, Quadruplets
- Fluidized Raft, Wake Aggregates

TWO PHASE FLOW MODELS FOR VISCOELASTIC FLUIDS ESSENTIALLY DO NOT EXIST

We get ideas and test ideas about modeling the interaction of forces needed for LNS and mixture theories from DNS.

SAND TRANSPORT IN FRACTURED RESERVOIRS



In a slot problem a particle laden (say 20% solids) fluid is driven by a pressure gradient and the particles settle to the bottom as they are dragged forward. Sand deposits on the bottom of the slot; a mound of sand develops and grows until the gap between the top of the slot and the mound of sand reaches an equilibrium value; this value is associated with a critical velocity. The physical processes here are *settling* and *washout.*Washout could be by sliding and slipping; however, a more efficient transport mechanism is by *advection after resuspension* which we studied by direct simulation.

Microstructural properties important for advection after resuspension include:

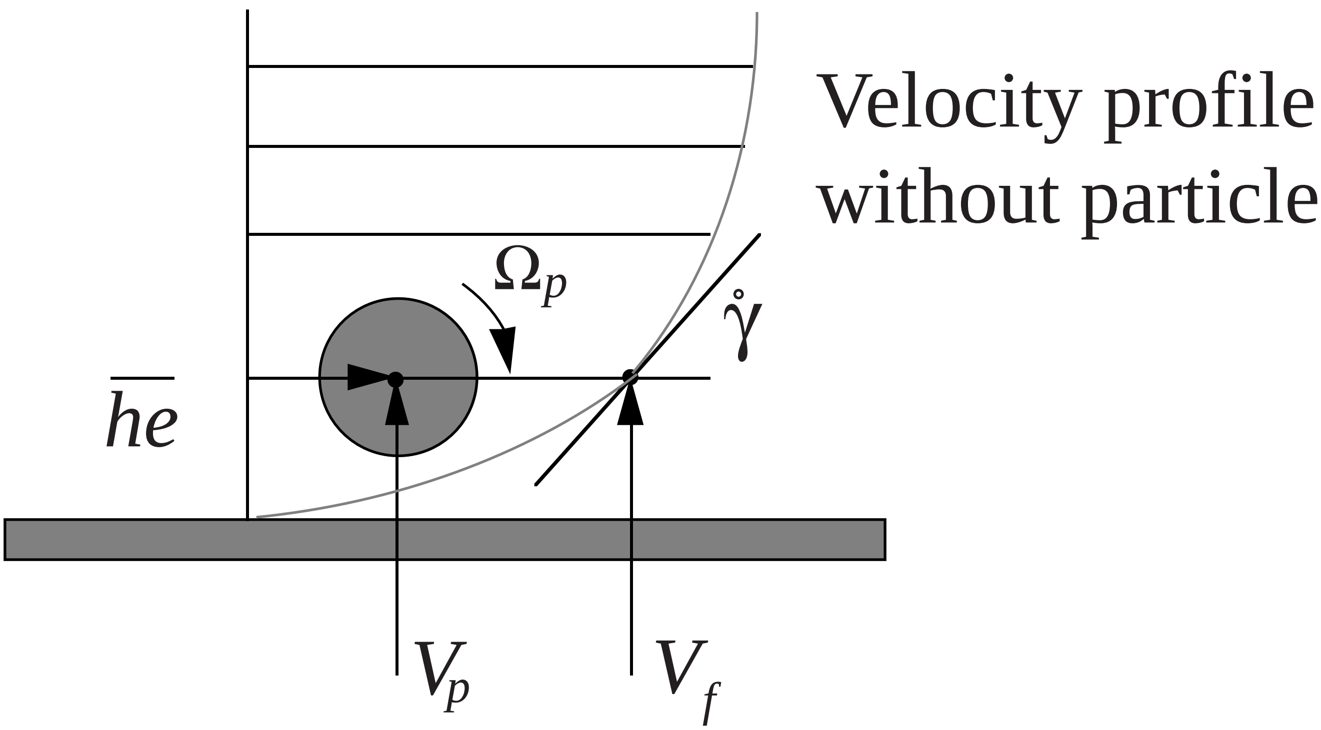
- **Lift-off**
- **Lift force minus weight**
- **Equilibrium height**
- **Slip velocities**

LIFT OFF or RESUSPENSION

A particle rests on a wall under a gravity. A Poiseuille flow is started. The particle slides and rolls on the bottom. At a certain speed or Reynolds number the particle lifts off and rises to an equilibrium height h_e where it is in balance under weight and lift as it moves forward and rotates. We computed these things using DNS.

ρ_p / ρ_f	Lift off *Re*
1.001	0.33
1.01	2.83
1.4	25

SLIP VELOCITY OF A PARTICLE



$(V_p, V_f) =$ particle velocity, fluid velocity

$V_f - V_p =$ slip velocity

$\mathring{\gamma}/2 - \Omega_p =$ angular slip velocity

Richardson-Zaki correlations

$$V_f - V_p = \Delta V_o \; f(c)$$

ΔV_o: Slip velocity for a single particle

$f(c)$: function of the concentration of solids

ΔV and $f(c)$ can be determined by experiments or DNS

LIMITATIONS OF DNS

These simulations complement and compete with experiments. Experiments tell the truth in all detail. The simulations, though potentially exact, have limitations of various kinds.

- **Number of particles.** Simulations of flows of hundreds of spheres in 2D and thousands in 3D have been achieved. We are hoping to move 100,000 particles in 2D and thousands in 3D
- **Collisions.** It is not possible to simulate the motion of even a moderately dense suspension of particles without a strategy to handle cases in which particles touch. Four strategies have been proposed and they work but they keep the particles farther apart than they ought to be, resulting in too high void fraction. An optimal strategy for collisions is an important and difficult challenge for DNS.

- **Turbulence.** No one has yet figured out how to do DNS when particles are in the fluid.
- **Viscoelastic fluids.** Even without particles these simulations can't be carried out at the high Weissenberg numbers frequently encountered in applications.

SINCE THE HORIZONS FOR DNS OF MULTIPHASE FLOW ARE NOT IN VIEW, WE CAN STRIVE TO ELIMINATE THESE LIMITATIONS ONE BY ONE.