# *Simulations of Particle-Fluid Suspensions with the Lattice-Boltzmann Equation*

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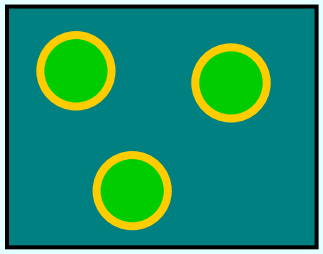
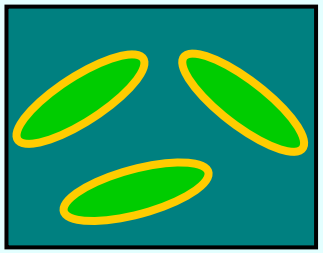
## *Derive a variety of micromechanical models of complex fluids from same basic ingredients*



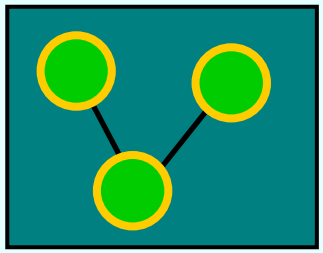
Colloids

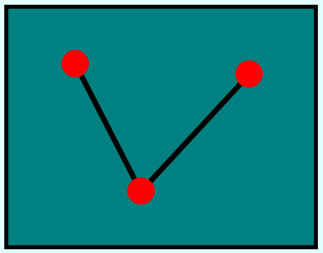


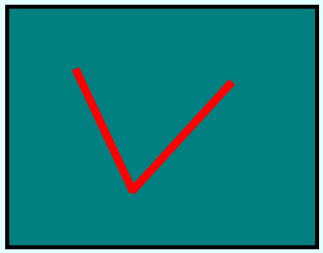
Liquid crystals

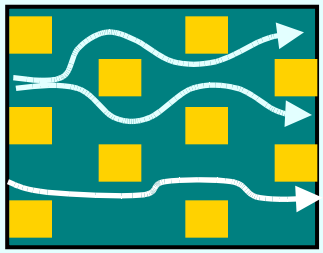
1. Solid particles-Newtonian Mechanics
2. Continuum fluid-Navier-Stokes equations
3. Stick boundary conditions couple particles and fluid.Valid for particles > 30nm (Add: charge, chemical bonds, inertia)

Computational framework for HI in a wide range of **materials**, **flows**, and **scales**.









Solutions of polymers and biopolymers

Porous Media

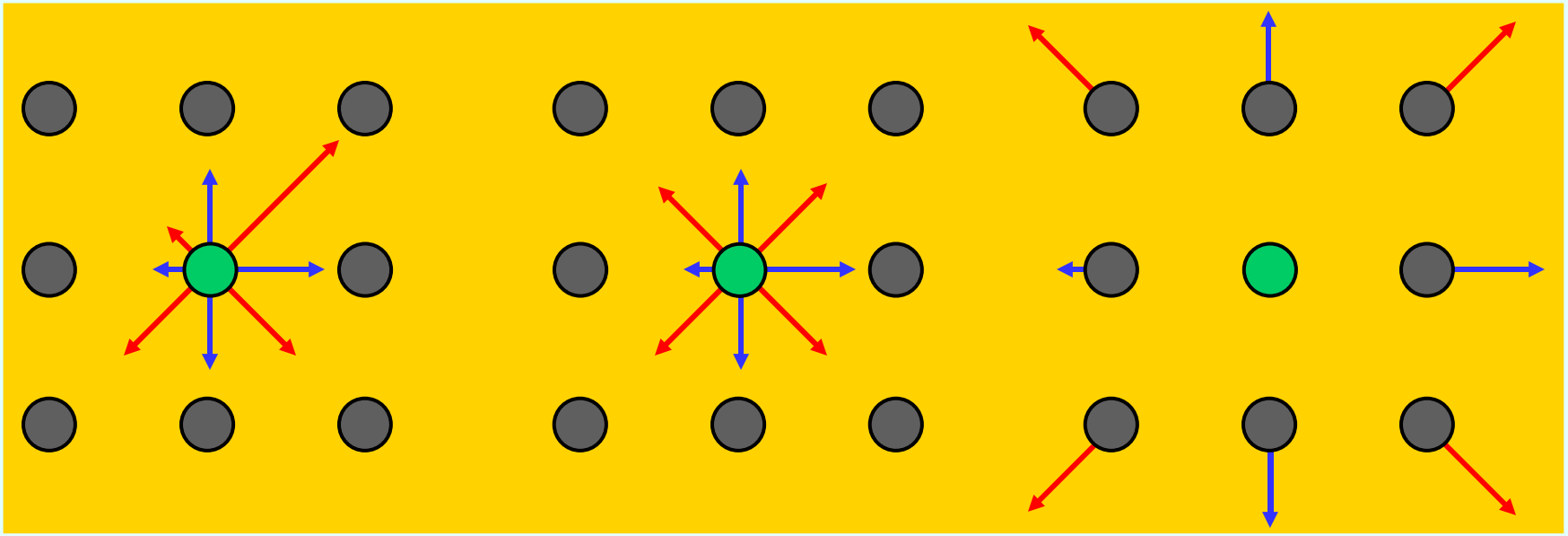
# *Outline: Applications of DNS to suspensions and particle fluid systems*

- Lattice-models for fluid dynamics
- Lattice-Boltzmann method
- 3 examples
  - Settling of particle clusters at small Re
  - Reactive flows in porous media (Stokes flow)
  - Polymer solutions (with Brownian motion)
- Closing thoughts

# *Lattice-gas models for suspensions*

- Lattice-gas models were introduced to simplify kinetic theory (Square lattice-HPP)
- FHP (‘86) showed that a hexagonal lattice gas could solve Navier-Stokes equations in 2D.
- LCF (‘88) used the FHP model to calculate viscosity and self-diffusion in a 2D colloidal suspension
- Projected 4D FCHC model for 3D simulations (Henon ’87)
- Moving boundary condition (FL ’89)
- Hydrodynamic interactions (LF ’90)
- But: LG models are too noisy; Sc ~ 1: Not Galilean invariant
- LBE (HS-with linearized collision operator)

# *LBE model introduces a discrete velocity distribution: local collisions and propagation*



Initial State:
x momentum
+ xy shear stress:

Post-Collision:
x momentum only

Propagation

$$n_i(\mathbf{r}+\mathbf{c}_i\Delta t, t+\Delta t) = n_i(\mathbf{r},t) - [n_i(\mathbf{r},t) - n_i^{EQ}(\mathbf{r},t)]/\tau$$

## *Hydrodynamic fields are moments of the discrete velocity distribution $n_i(\mathbf{r},t)$*

$$\rho(\mathbf{r},t) = \sum_{i=0}^{18} n_i(\mathbf{r},t) \qquad \text{Mass}$$

$$\rho(\mathbf{r},t)\mathbf{u}(\mathbf{r},t) = \sum_{i=0}^{18} n_i(\mathbf{r},t)\mathbf{c}_i \qquad \text{Momentum}$$

$$p(\mathbf{r},t) + \rho(\mathbf{r},t)\mathbf{u}(\mathbf{r},t)\mathbf{u}(\mathbf{r},t) = \sum_{i=0}^{18} n_i^{EQ}(\mathbf{r},t)\mathbf{c}_i\mathbf{c}_i \qquad \text{Euler Stress}$$

$$\sigma(\mathbf{r},t) = -\sum_{i=0}^{18}\left[ n_i(\mathbf{r},t) - n_i^{EQ}(\mathbf{r},t) \right]\mathbf{c}_i\mathbf{c}_i \qquad \text{Viscous Stress}$$

3D model has 19 velocities $\mathbf{c}_i$: 000, 100 & 110 directions

# *Macrodynamic behavior from Chapman-Enskog analysis*

$$\sum_i n_i(\mathbf{r}+\mathbf{c}_i\Delta t, t+\Delta t)\mathbf{c}_i^n = \sum_i n_i(\mathbf{r},t)\mathbf{c}_i^n - \sum_i \frac{[n_i(\mathbf{r},t)-n_i^{EQ}(\mathbf{r},t)]}{\tau}\mathbf{c}_i^n$$

Define macroscopic length and time scales:

$$n_i = n_i^{eq} + \varepsilon n_i^1; \quad \mathbf{r}_1 = \varepsilon\mathbf{r}; \quad t_1 = \varepsilon t; \quad t_2 = \varepsilon^2 t$$

Equilibrium distribution is *chosen* to give correct Euler stresses (Same low-order moments as Maxwell-Boltzmann distribution)

$$n_i^{EQ}(\rho,\mathbf{u}) = a^{c_i}\left[\rho + \frac{\rho\mathbf{u}\cdot\mathbf{c}_i}{c_s^2} + \frac{\rho\mathbf{u}\mathbf{u}:\left(\mathbf{c}_i\mathbf{c}_i - c_s^2\mathbf{1}\right)}{2c_s^2}\right]$$

# *Expand space and time derivatives to 2nd order and collect terms*

To first order: $\partial_{t_1}\rho + \nabla_1\left(\rho\mathbf{u}\right) = 0 \qquad n=0$

$$\partial_{t_1}\left(\rho\mathbf{u}\right) + \nabla_1\left(\rho c_s^2 + \rho\mathbf{u}\mathbf{u}\right) = 0 \qquad n=1$$

$$\partial_{t_1}\left(\rho c_s^2 + \rho\mathbf{u}\mathbf{u}\right) + \nabla_1\left(\rho c_s^2\mathbf{u}\mathbf{I}\right) = \frac{\sigma_1}{\tau} \qquad n=2$$

$$\sigma_1^c = \rho c_s^2\tau\left[\left(\nabla_1\mathbf{u}\right) + \left(\nabla_1\mathbf{u}\right)^T\right]$$

To 2nd order:

$\partial_{t_2}\rho = 0$ Incompressible on $t_2$ scale

$$\partial_{t_2}\left(\rho\mathbf{u}\right) + \left(\Delta t/2\right)\nabla_1\left(\rho c_s^2\left(\nabla_1\mathbf{u}\right) + \rho c_s^2\left(\nabla_1\mathbf{u}\right)^T\right) = \nabla_1\cdot\sigma_1$$

"Lattice viscosity"-eliminates grid diffusion

# *Lattice-Boltzmann approximates Navier-Stokes on "large" scales*

Combining results from different time scales:

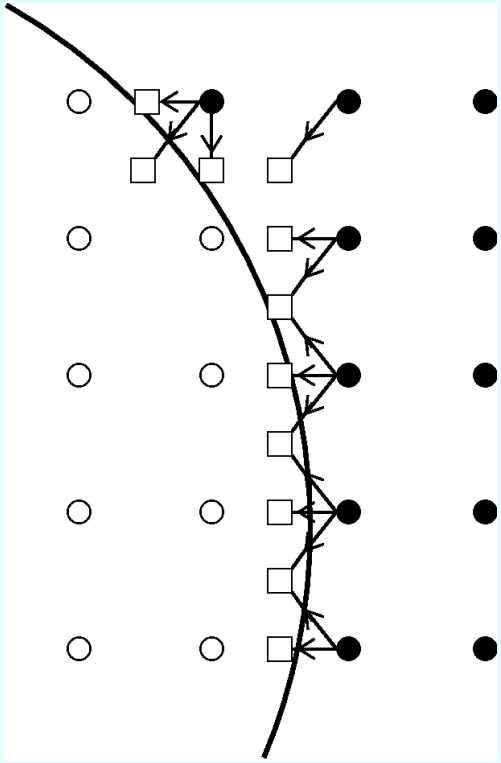
$$\partial_t \rho + \nabla \cdot \left( \rho \mathbf{u} \right) = 0$$

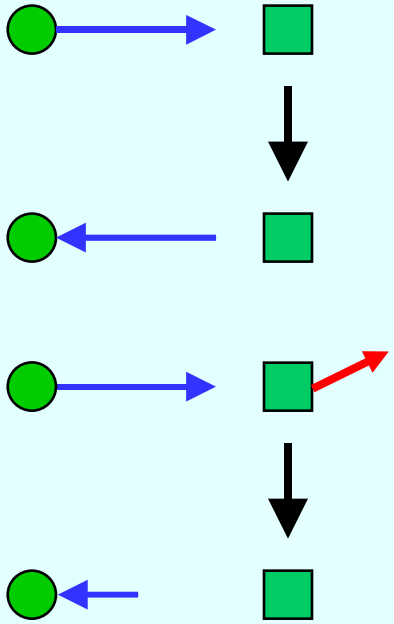
$$\rho \partial_t \mathbf{u} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \eta \left[ \nabla^2 \mathbf{u} + \nabla \nabla \cdot \mathbf{u} \right]$$

$$p = \rho c_s^2; \quad c_s^2 = \frac{1}{3} \frac{\Delta x^2}{\Delta t^2}; \quad \eta = \left( 2\tau - 1 \right) \rho c_s^2 \Delta t$$

Navier-Stokes fluid dynamics in low velocity limit $M < 0.3$
Leading order errors are $M^2$ and $\Delta x^2$.

# *Moving boundary condition by additional mass transfer-continuously varying velocity*





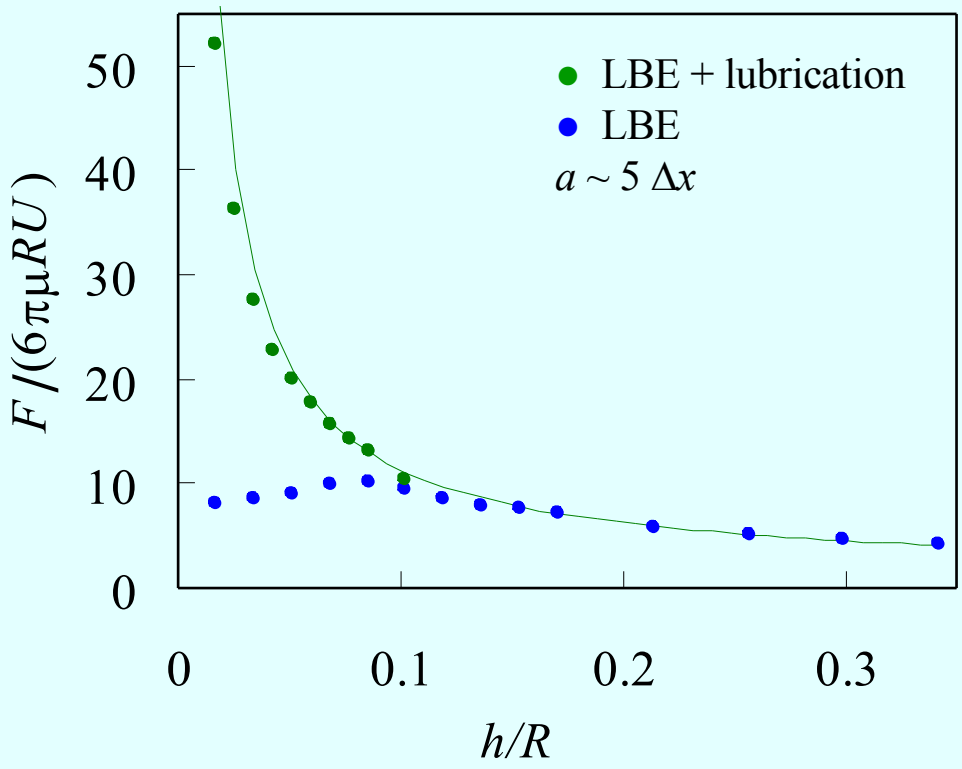
Stationary Boundary

Moving Boundary

$\Delta n \propto \mathbf{u} \cdot \mathbf{c}_i$

Mass transfer prevents artificial pressure gradients
Boundary conditions conserve global fluid mass
Momentum transferred into particle forces and torques

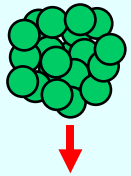
# *Lubrication forces important in dense suspensions; dominant in shear flows*




- Impractical to resolve flow in gap by any multi-particle method: grid based, multipole, or boundary element.
- Add lubrication forces pair by pair
- Single patch point ~ $0.5\Delta x$
- Similar results for other components of $F$ & $T$
- 2 additional patch points (independent of $a$)

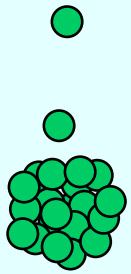
# *Settling of a cluster of particles shows strong inertial effects even for Re ~ 1.*

Cluster of 100-1000 particles $\mathrm{Re}_c = \dfrac{2\rho U_c R_c}{\mu}$



a) $\mathrm{Re}_c < 1$: Cluster maintains shape

Gradually sheds particles

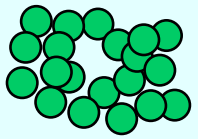


Batchelor & Nitsche

b) $\mathrm{Re}_c > 1$: Forms ring structure

No shedding of particles

Breaks into smaller rings (Nicolai)



# *Computational details*

1812 particles: diameter 5.4 $\Delta x$: $R_c \sim 15a$ : $\varphi \sim 0.55$: $\mathrm{Re}_c \sim 5$

Periodic unit cell: 1024 x 400 x 400

~160 million grid points; 100,000 steps

16 P4 Xeons connected by Gigabit ethernet: 32 cpu's

32 MSUPS aggregate performance: Run time ~150 hours

New cluster: 192 dual-core P4's with Gigabit ethernet

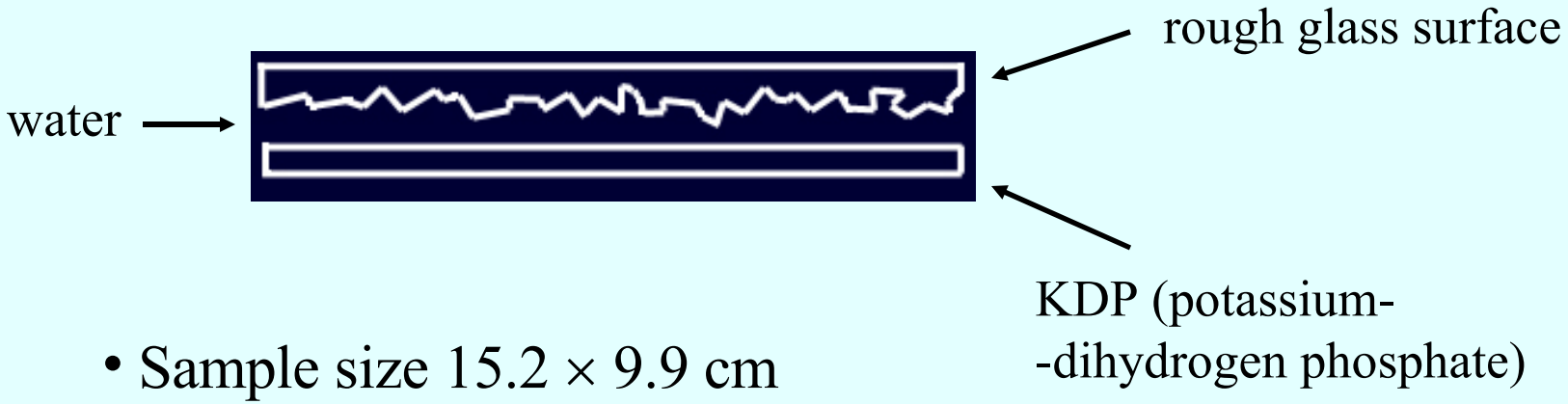
Observed good scaling up to 96 processors (~300 MSUPS)

But still only limited inter-switch bandwidth (20Gbits/sec)

Good scaling requires high performance switch

Extreme Networks x450a-48t ($6500)

# *Dissolution in a rough fracture. Modeling experiments by Detwiler et al., (GRL 2003)*




- Sample size 15.2 × 9.9 cm
- Initial mean aperture $\langle h_0 \rangle = 0.126$ mm
- dissolved until $\langle h \rangle = 2\langle h_0 \rangle$ at Pe = 54 and Pe = 216
- high resolution data on fracture topography

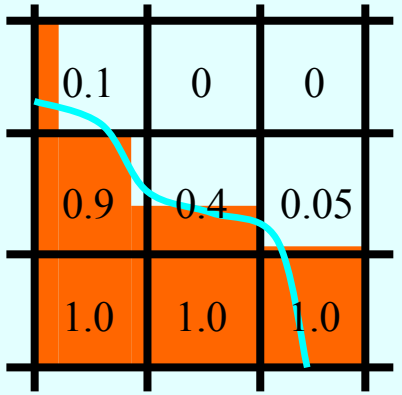
# *Velocity field calculated from implicit LBE*

3D Stokes equations $\begin{cases} \nabla \cdot \mathbf{v} = 0 \\ \eta \nabla^2 \mathbf{v} = \nabla p \end{cases}$

- Sub-grid scale boundary conditions

- Steady-state solution determined directly, using conjugate gradients

(Verberg, Ladd, 2000)

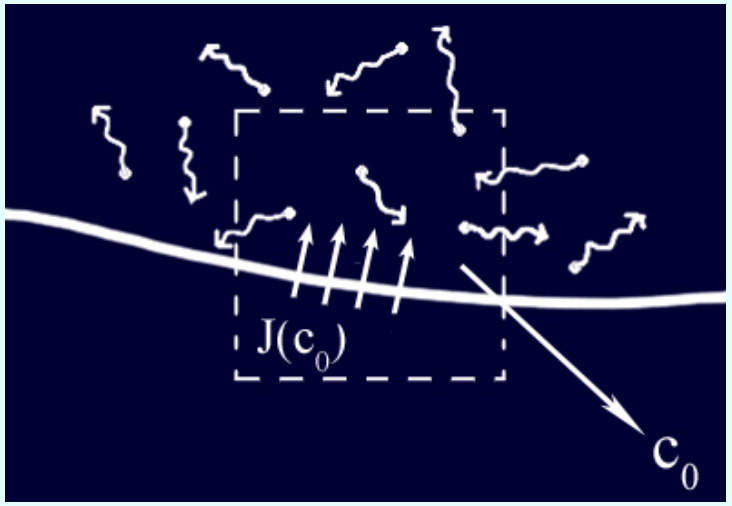



more than 2 orders of magnitude faster than standard LBE

# *Random walk improvements*

Classical random walk:

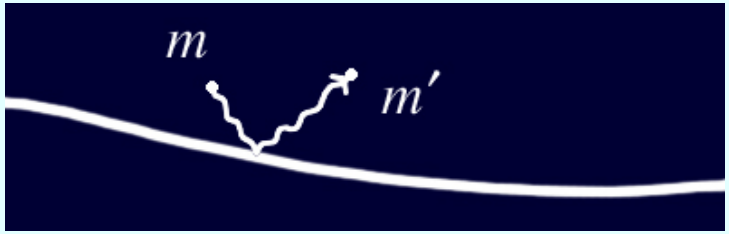
$\sim 10^3$ particles per cell needed for accurate calculation of $J(c_0)$




Variable mass random walk:

- Tracking one particle at a time
- Works for linear kinetics only

$$J = k(c_s - c_0)$$

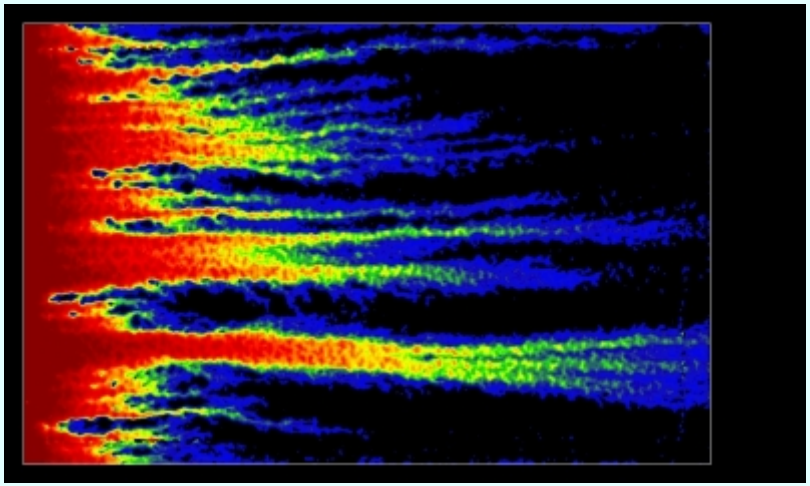



$$\frac{m'}{m} \neq 1$$

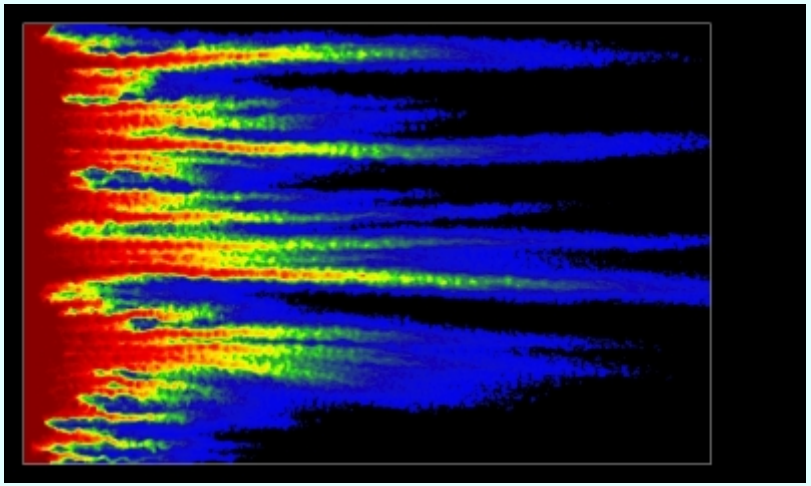
# *Aperture growth at Pe = 54*

$\langle h \rangle = 2\langle h_0 \rangle$

experiment



simulation



$7\langle h_0 \rangle$

0

- Channels form, grow, and compete for the flow
- Only a few channels survive at the end
- Strongly non-linear process

# *Key problem in simulating polymer solutions is the very long time scales.*

Characteristic polymer relaxation time

$$\tau_Z \sim \left( R_G / b \right)^3 \tau_M = N^{1.8} \tau_M ; \quad \tau_M = b^2 / D_M$$

For 100 unit chain, $10^2$ steps per monomer diffusion time

$\sim 10^6$ steps per Zimm time

Need a short cycle time ($< 10^{-3}$s) to permit useful simulations of long-chains.

Brownian dynamics restricted to chains < 100 monomers since cycle time is proportional to $N^3$

Use point particles to obtain a polymer simulation method

Inertial equivalent of Brownian dynamics.

# *Brownian motion can be added to LBE via fluctuations in fluid stress (controlled)*

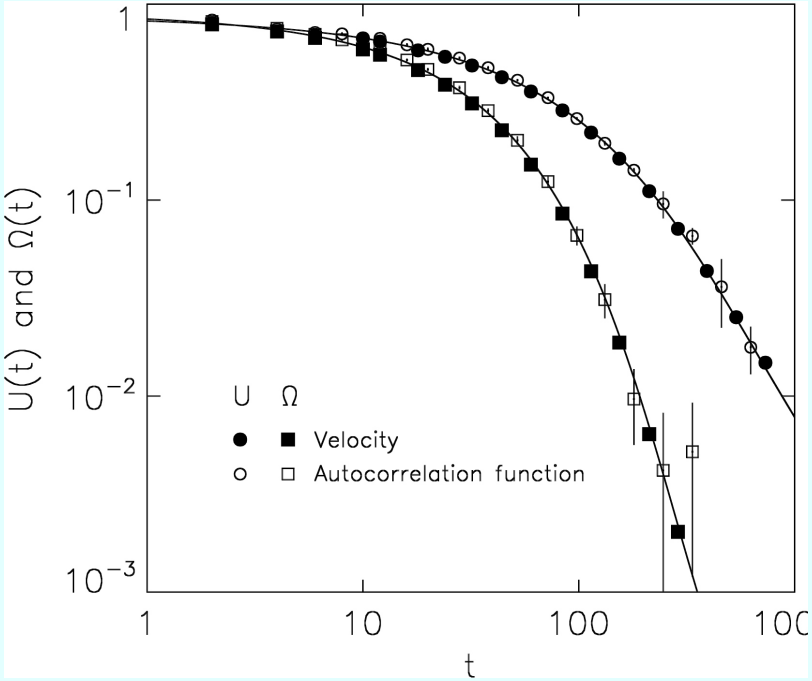
Add Gaussian white noise at each node

$$n_i(\mathbf{r}+\mathbf{c}_i\Delta t, t+\Delta t) = n_i(\mathbf{r},t) - [n_i(\mathbf{r},t) - n_i^{EQ}(\mathbf{r},t)]/\tau + n_i^f$$

So that the fluctuation dissipation relation is satisfied

$$\left\langle \left(\sigma_{xy}^f\right)^2 \right\rangle = 2\mu k_B T; \quad \sigma_{xy}^f = \sum_{i=0}^{i=18} n_i^f c_{i,x} c_{i,y}$$

Velocity correlation function of a suspended particle agrees quantitatively with dissipative decay of velocity and with Boussinesq equation



# *Collision operators for MRT, M10, BGK*

$$m_k = \sum_{j=0}^{N_b} e_{k,j} n_j$$

$$m_k' = m_k^{eq} + (1+\lambda_k) m_k^{neq} + m_k^e + m_k^f$$

$$m_0^{eq} = \rho; \quad m_{1-3}^{eq} = \rho \mathbf{u}; \quad m_{4-9}^{eq} = \rho c_s^2 + \rho \mathbf{uu}$$

$$m_0^e = 0; \quad m_{1-3}^e = \mathbf{f}; \quad m_{4-9}^e = \mathbf{uf} + \mathbf{fu}$$

$$m_0^f = 0; \quad m_{1-3}^f = 0; \quad m_{4-9}^f \sim \sqrt{2\eta T}$$

$$m_{10-18}^{eq} = m_{10-18}^e = 0; \quad m_{10-18}^f \sim \sqrt{2\eta T}$$

$$n_i(\mathbf{r} + \mathbf{c}_i \Delta t, t + \Delta t) = w_i \sum_{k=0}^{N_b} m_k'(\mathbf{r}, t) \frac{e_{k,i}}{\mathbf{e}_k \cdot \mathbf{e}_k}$$

$$e_0 = 1$$
$$e_1 = c_x$$
$$e_2 = c_y$$
$$e_3 = c_z$$
$$e_4 = c^2 - 1$$
$$e_5 = 2c_x^2 - c_y^2 - c_z^2$$
$$e_6 = c_y^2 - c_z^2$$
$$e_7 = c_y c_z$$
$$e_8 = c_z c_x$$
$$e_9 = c_x c_y$$

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$$e_{10} = (3c^2 - 5)c_x$$
$$e_{11} = (3c^2 - 5)c_y$$
$$e_{12} = (3c^2 - 5)c_z$$
$$e_{13} = (c_y^2 - c_z^2)c_x$$
$$e_{14} = (c_z^2 - c_x^2)c_y$$
$$e_{15} = (c_x^2 - c_y^2)c_z$$
$$e_{16} = 3c^4 - 6c^2 + 1$$
$$e_{17} = (2c^2 - 3)(2c_x^2 - c_y^2 - c_z^2)$$
$$e_{18} = (2c^2 - 3)(c_y^2 - c_z^2)$$

# *Collision operators and hydrodynamic size*

$\lambda_k = 0$ for $k = 0, 1, 2, 3$: conservation laws

MRT: six independent, non-zero $\lambda_k$ (by symmetry)

Adjust location of hydrodynamic boundary via $\lambda_{10\text{-}18}$.

M10: three $\lambda_k$; $\lambda_k = -1$ for $k > 9$.

BGK: one $\lambda_k$; all $\lambda_k$ equal (for $k > 3$).

- MRT: $\tau$-independent radius ($a_0 = 2.7$).
- Decreased computational time, since large viscosity now accessible
- Insignificant differences in speed 1250 ticks/site (P4)

| τ | BGK | M10 | MRT |
|---|---|---|---|
| 0.53 | 2.77 | 2.94 | 2.73 |
| 0.55 | 2.73 | 2.90 | 2.72 |
| 0.6 | 2.75 | 2.83 | 2.71 |
| 0.7 | 2.69 | 2.77 | 2.71 |
| 1 | 2.58 | 2.67 | 2.72 |
| 2 | 1.90 | 2.45 | 2.70 |
| 5 | 1.04 | 2.09 | 2.69 |
| 10 | 0.43 | 1.73 | 2.67 |

# *Fluctuations*

Fluctuations in stress (Landau): $\left\langle \left( m_7^f \right)^2 \right\rangle = \left\langle \sigma_{yz}^2 \right\rangle = 2T\eta\lambda_7^2$

$\lambda_7$ corrects for discrete time FDT

Improved agreement with FDT by including fluctuations in $m_{10\text{-}18}$ (Adhikari et al., 2004).

$$\frac{\left\langle j_x^2 \right\rangle}{\rho T} \sim 0.6 - 0.8; \quad \text{stress fluctuations only}$$

$$\frac{\left\langle j_x^2 \right\rangle}{\rho T} = 1; \quad \text{including fluctuations in } m_{10-18}$$

# *Point forces couple polymer and fluid (Ahlers and Duenweg ~2000)*

For a bead-rod or bead-spring chain + fluctuating LBE fluid:

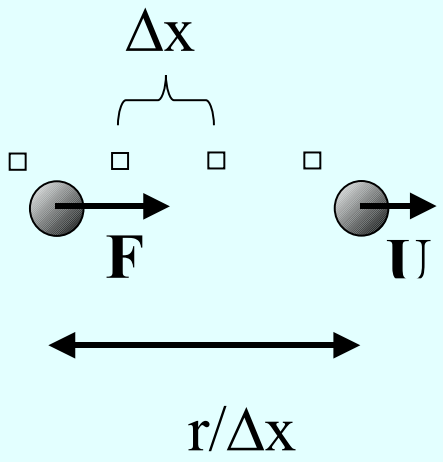
2) Calculate velocity field at each bead by interpolation
3) Calculate force on bead based on velocity relative to fluid
4) Redistribute force to LBE nodes
5) Add fluctuating force to beads to balance frictional losses

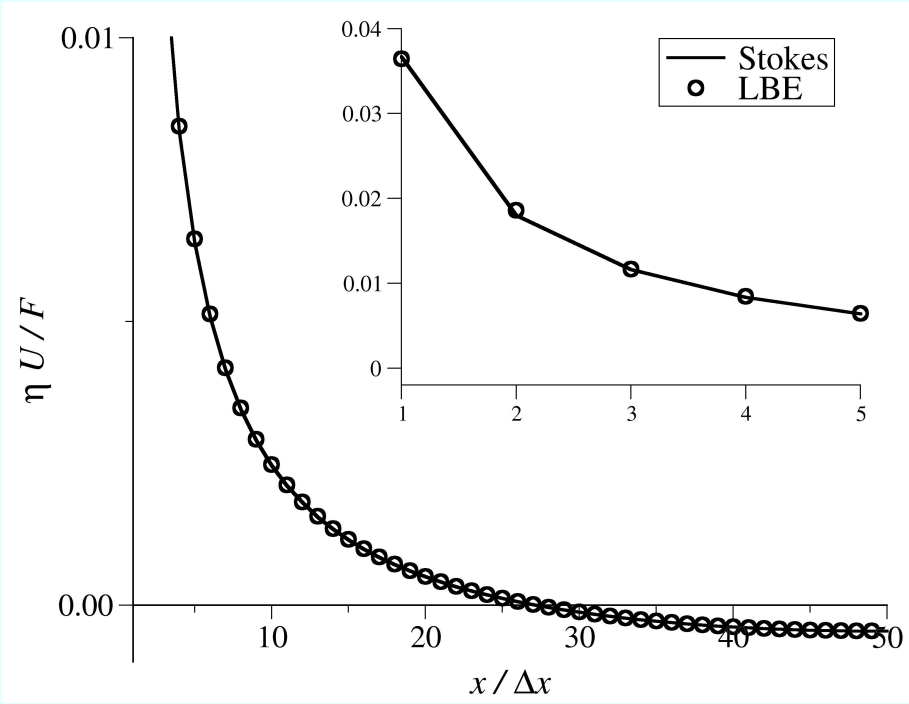
Single particle correlation matrix

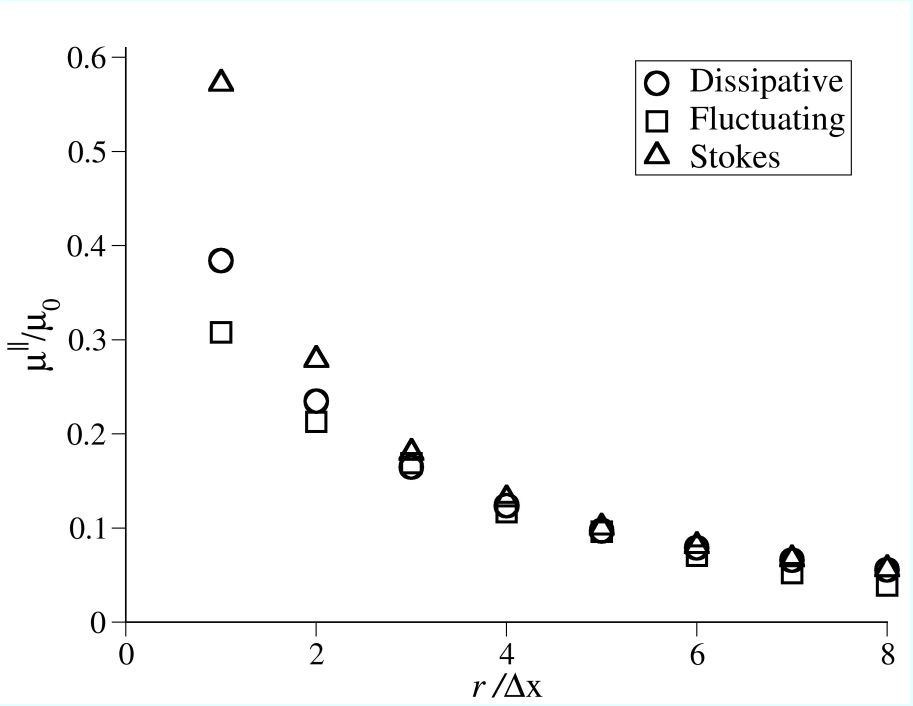
Long-range correlations in random force come from fluid dynamics of fluctuating LBE model.

Studied dynamical scaling laws in long chains ($N \sim 10^3$) but for relatively short times.

# *Hydrodynamic Interactions between point particles*



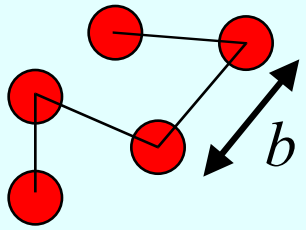



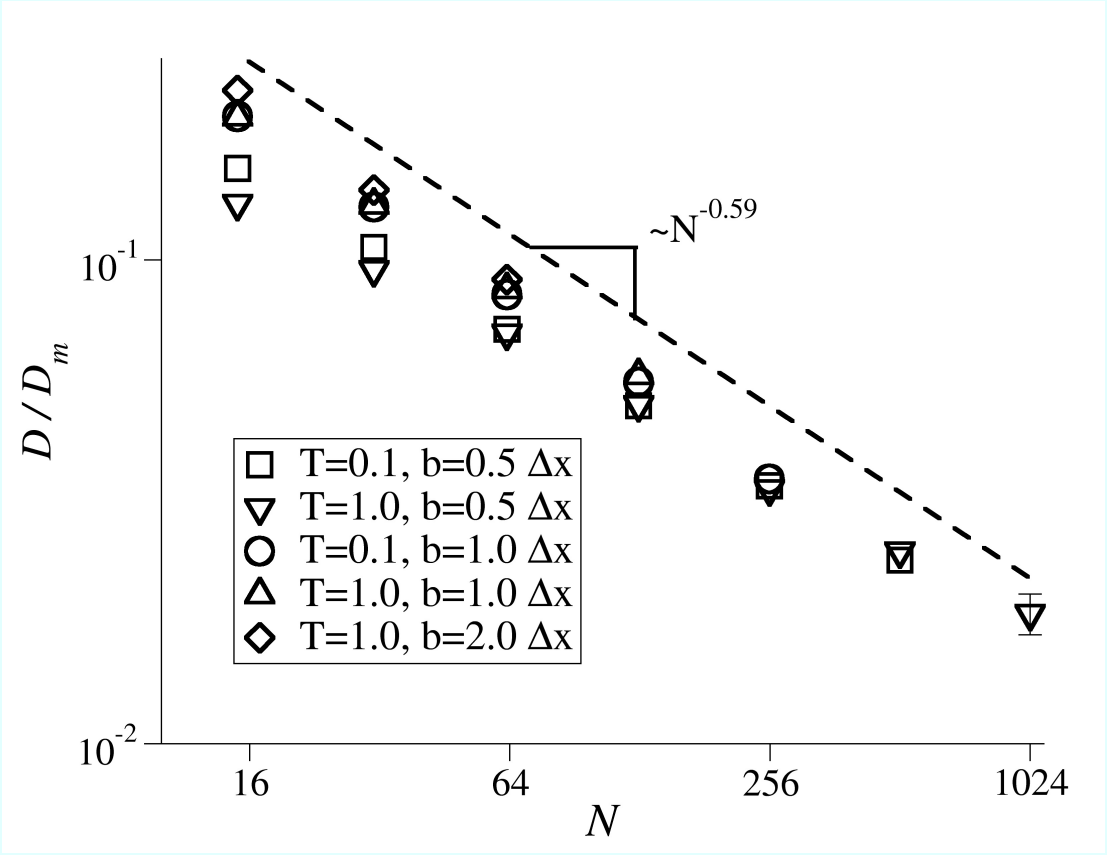




On lattice

Off lattice

# *Self-diffusion of an isolated chain*




$$V \sim N^{1.8} b^3$$

$$t_Z \sim N^{1.8} b^3 \eta / T$$

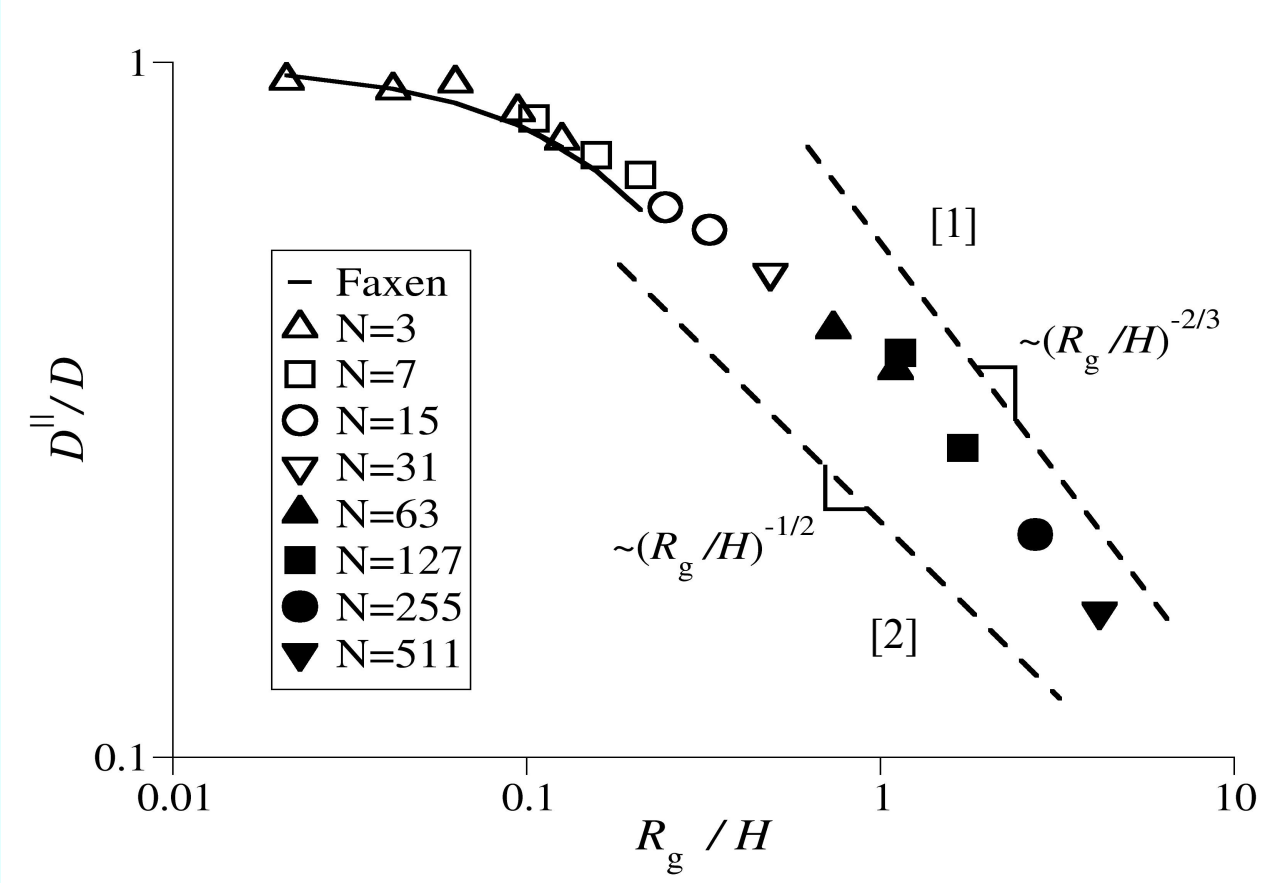
$$\text{CPU TIME} \sim N^{3.6} b^6 / T$$

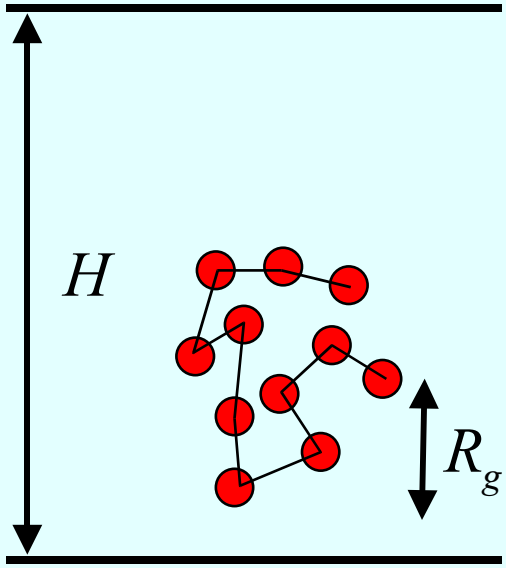
Computational effort can be greatly reduced for longer chains.

Fixed $R_g \sim 5\Delta x$

Independent of $N$.

# *Self-diffusion of an confined polymer*





[1]Brochard F, deGennes P G, *J. Chem. Phys.*, **67**,52

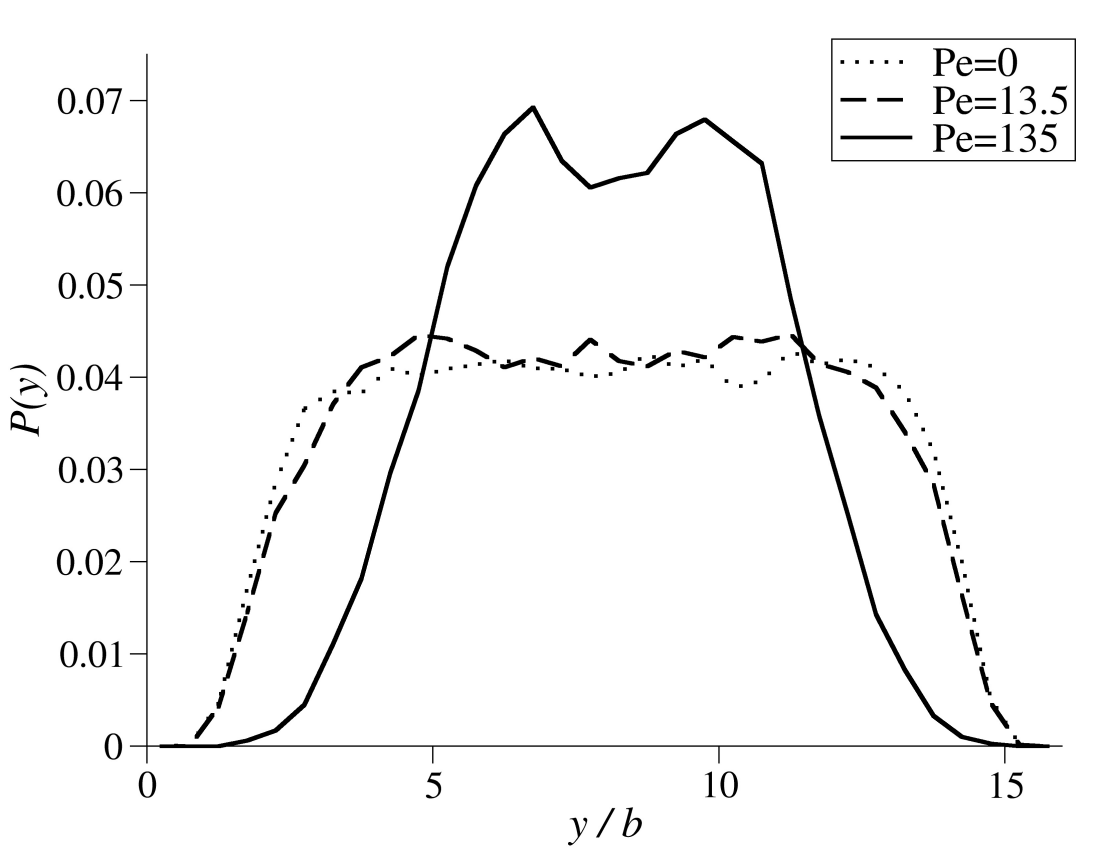
[2]Jendrejack et al., *J. Chem. Phys.*, **119**,1165

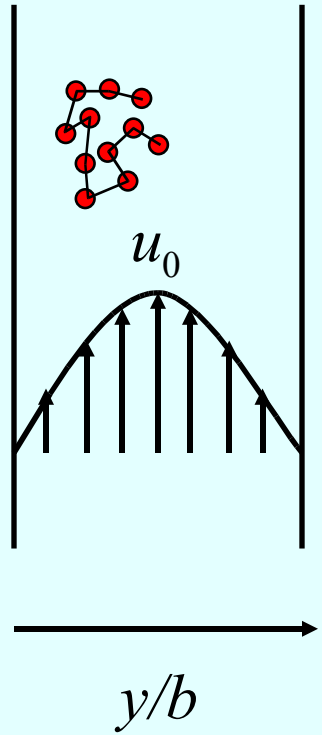

**Weak Confinement** ⟵

**Strong Confinement** ⟶

# *Confined polymers in flow*

$$N = 15 \qquad H \sim 8R_g \qquad Pe = \frac{4u_0 R_g^2}{DH}$$



# *Particle methods fall into two categories*

| | | |
|---|---|---|
| Forces: | MD | Conservative |
| | DPD | Conservative, Dissipative, Fluctuating |
| | SPH | Conservative, pressure (from EOS) |

Computationally intensive neighbor search ~ 1000 FLOP

| | | |
|---|---|---|
| Collisions: | DSMC | Boltzmann |
| | LG | Discrete |
| | RCLG | Rotational |

Local collision process is faster but only applicable to gases.
Spatial resolution limited by cell size

# *Particle methods are not competitive with CFD or LBE for hydrodynamic problems*

Statistics: $u_{max} < 0.3\ c_s$ to maintain incompressibility

10% accuracy requires ~ 1000 particles

Maximum resolution ~ 10 particles

Computational effort $10^4$-$10^5$ larger than CFD

Time averaging means reducing $u_{max}$

Time scales: $$Sc = \frac{\tau_D}{\tau_H} = \frac{\eta/\rho}{D} \sim \frac{\eta/\rho}{k_B T/\eta a} \sim \frac{a}{\sigma} \qquad \left(\eta \sim \frac{\sqrt{m k_B T}}{\sigma^2}\right)$$

Cannot enforce proper time scale separation unless $a \gg \sigma$ (of the order of 1000 in colloids)

SPH and DSMC used for large-scale, high-speed flows

# *Even DPD does not work well for HI*

Dissipative forces can increase $Sc \sim 1.6 \times 10^{-5} \tilde{\gamma}^2 \tilde{n}^3 a r_c^{-1}$

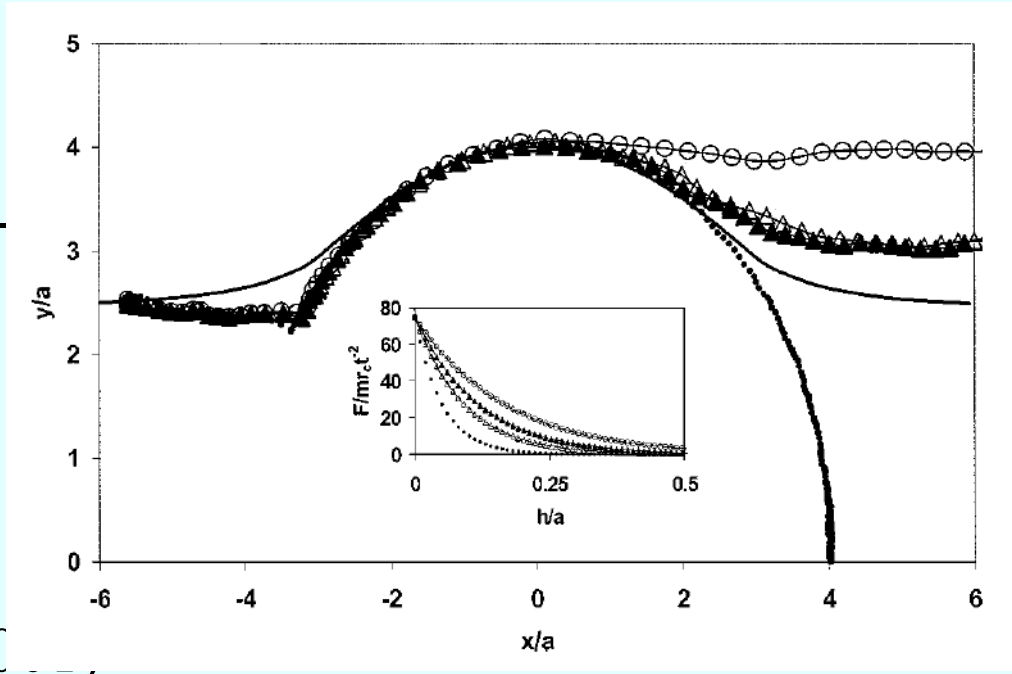
But needs very large friction, $\tilde{\gamma} \sim 100$

and density, $\tilde{n} \sim 10$

Depletion forces perturb thermodynamics and short-range structure

No hydrodynamics at small scales

(Whittle & Dickinson JCIS 20[illegible])



# *Some advantages of LBE*

External boundaries: arbitrary shape, no added cost

Simplicity of random forces; potentially very fast

Simplicity (<5000 lines) and speed ($10^{12}$ grid points/day)

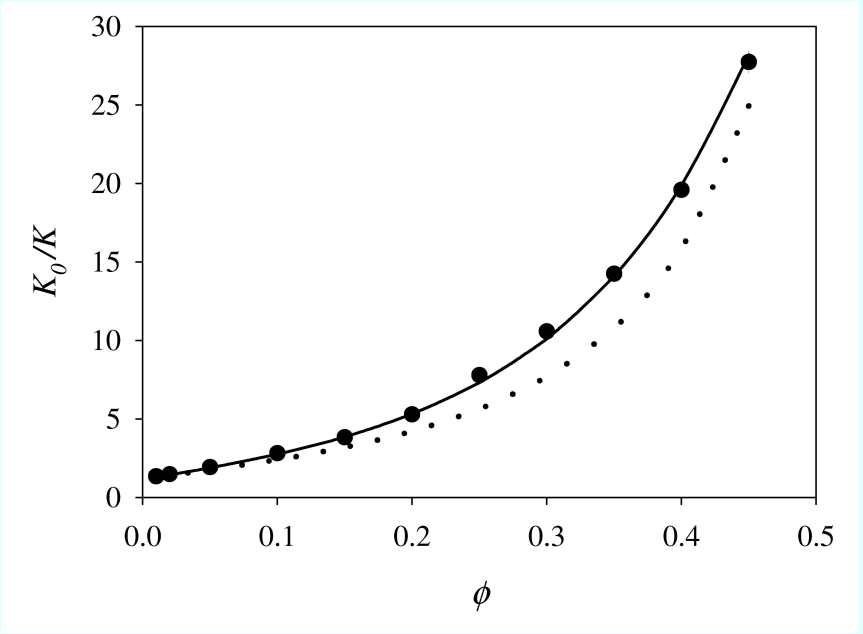
Superior accuracy for relative motion between solid and fluid

Permeability of random arrays of spheres ($N = 16$)

LBE: solid circles ($a = 2\Delta x$)

Multipole: solid line (M=200)

Brinkman: dotted line



# *Closing thoughts*

Discrete kinetic theory (LGA/LBE) developed from intuitive, physically based, models: HPP-FHP-HS

Led to numerically important constraints being built in

- Exact conservation laws
- Isotropic momentum diffusion (weighted diagonals)
- Dispersion free

Models developed from physically motivated guesses: e.g. Moving boundary condition from Monte Carlo

Past 10 years LBE has become increasingly mathematical

- Improved accuracy via unphysical equilibrium distribution
- Improved numerics: adaptive grids, elliptic solvers, etc.

But I believe there are still opportunities for physical insight.