Microhydrodynamics

Kengo Ichiki May 24, 2007

- 1. Multiple Scales
- 2. Hydrodynamic Interaction
- 3. Stokesian dynamics
- 4. Nanotechnology

1. Multiple Scales

Supramolecular **Nanomaterials Biomolecules** Nanocatalysts architectures Modeling on multiple scales OND Electronic Car-Parrinelo Molecular Model Continuum Structure Method Effective Medium Molecular simurations Quantum Chemistry Theories Monte Calro GB, PCM, COSMO Ab initio HF Ab initio KS-DFT Molecular Mechanics Energy and mass Semi-empirical Molecular Dynamics Transport Models Statistical Physics . Integral Equation Theories

[http://www.cein.ualberta.ca/research/nint/theory-modeling-group/research/index.html]

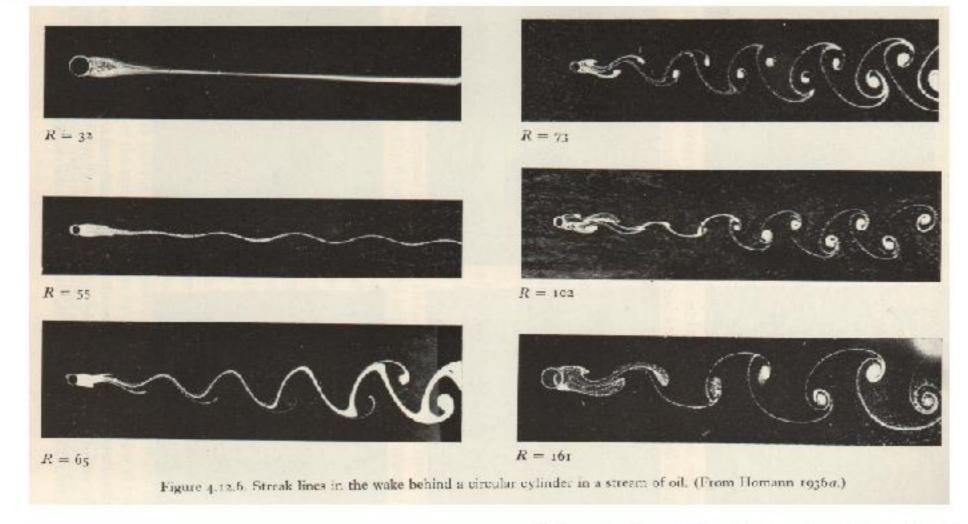
1. Multi-Scale in Fluids

Navier-Stokes eq.

$$\rho \Big(\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \boldsymbol{\nabla}) \boldsymbol{u} \Big) = -\boldsymbol{\nabla} p + \mu \nabla^2 \boldsymbol{u},$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0 \quad \text{(incompressible)}$$

Reynolds number : $Re = \frac{\rho LU}{\mu}$



[Batchelor "An Introduction To Fluid Dynamics"]

1. Multi-Scale in Particle Systems

Atoms/Molecules

Molecular dynamics

$$m{m} \cdot rac{\mathrm{d} m{U}}{\mathrm{d} t} = m{F} \qquad egin{matrix} \mathrm{intermolecular}, \ \mathrm{electrostatic}, \dots \ \mathrm{forces}. \end{split}$$

Dispersions

(colloids, polymers)

- Brownian dynamics
- Stokesian dynamics

Gnarular systems

Granular dynamics

Stars and Galaxy

Stellar dynamics

$$m{m} \cdot rac{\mathrm{d} m{U}}{\mathrm{d} t} = m{F}^{\mathrm{HI}} + m{F}^{\mathrm{B}} + m{F}^{\mathrm{ext}},$$

 $\boldsymbol{F}^{\mathrm{HI}}$: hydrodynamic interaction

$$= -R \cdot U$$

 \mathbf{F}^{B} : Brownian force

$$\overline{\boldsymbol{F}^{\mathrm{B}}(0)\boldsymbol{F}^{\mathrm{B}}(t)} = 2kT\boldsymbol{R} \ \delta(t)$$

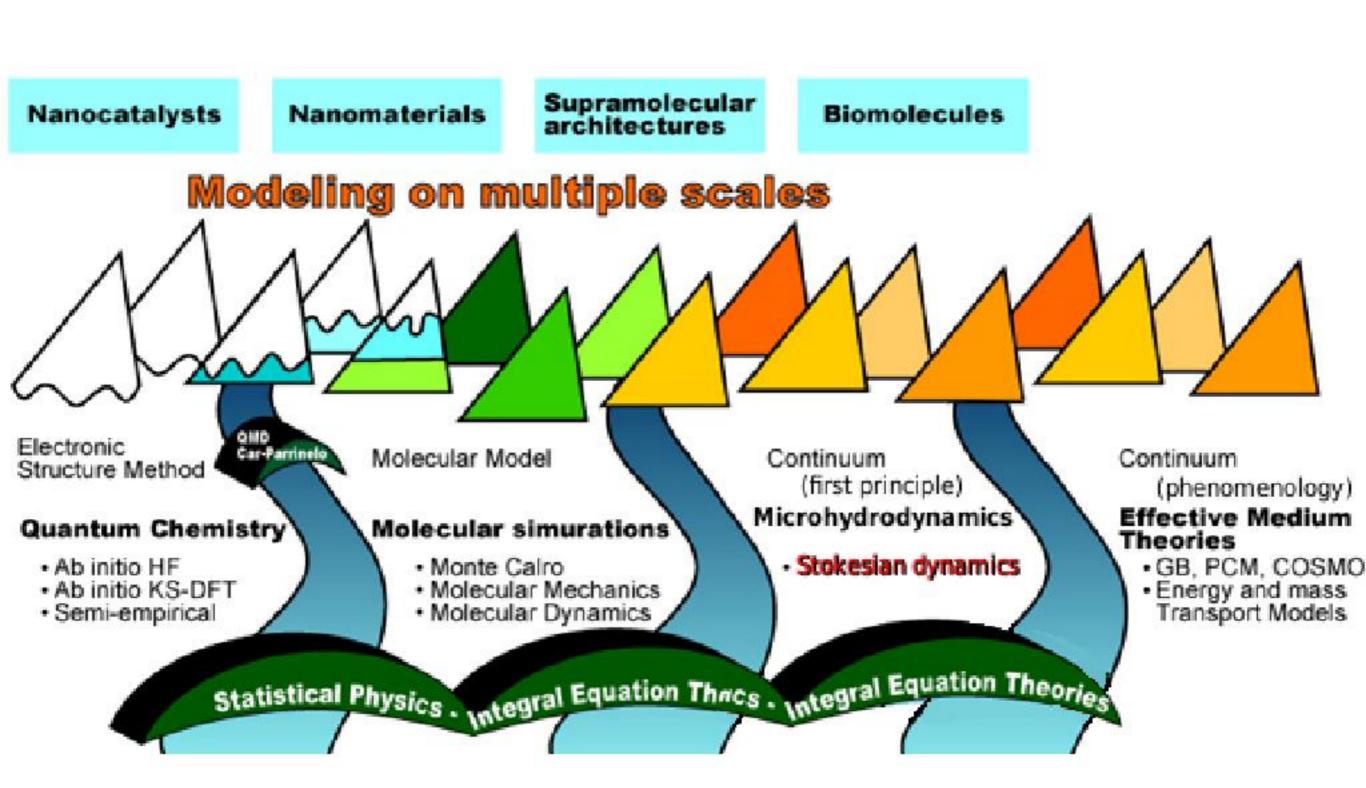
 F^{ext} : external force

for massless non-Brownian particles

$$\boldsymbol{R}\cdot\boldsymbol{U}=\boldsymbol{F}^{\mathrm{ext}}$$

1. Microhydrodynamics

"first-principle simulation for the continuum"



2. Hydrodynamic Interaction

Hydrodynamics

Stokes eq.

$$0 = -\nabla p + \mu \nabla^2 \mathbf{u},$$
$$\nabla \cdot \mathbf{u} = 0 \quad \text{(incompressible)}$$

point force

$$u(x) = \frac{1}{8\pi\mu} J(x - x_0) \cdot F_0$$

$$J(r) = \frac{1}{r} \left(I + \frac{rr}{r^2} \right)$$

Stokes drag

$$\mathbf{F} = 6\pi\mu a(\mathbf{U} - \mathbf{u}^{\infty})$$

Electrostatics

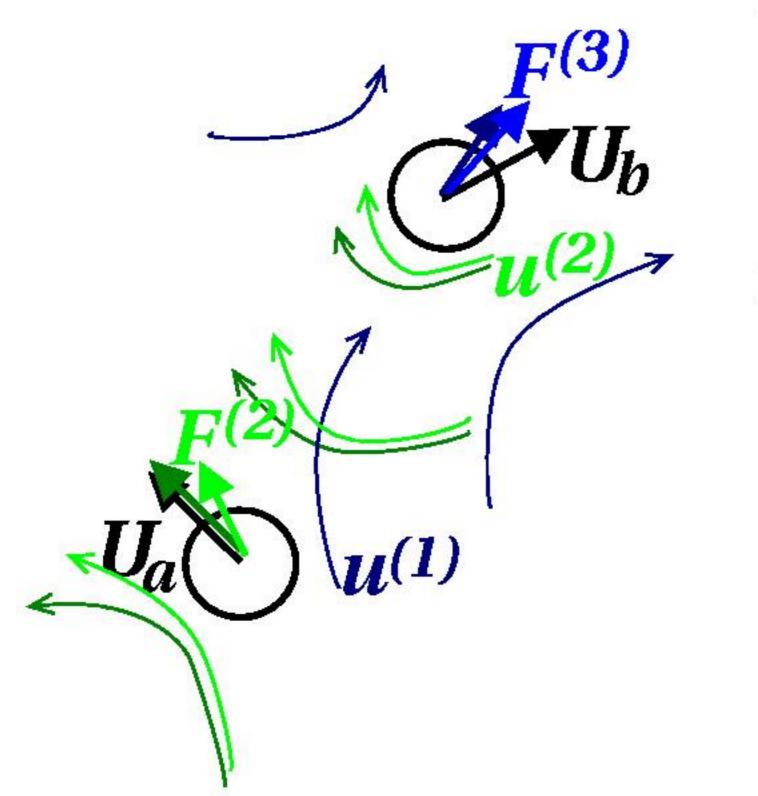
Poisson eq.

$$-\nabla^2 \phi = \frac{\rho}{\epsilon_0}$$

point charge

$$\phi(\boldsymbol{x}) = \frac{1}{4\pi\epsilon_0} G(\boldsymbol{x} - \boldsymbol{x}_0) \ \rho_0$$
$$G(\boldsymbol{r}) = \frac{1}{r}$$

2. Many-Body Interaction



place particle "a"

$$\boldsymbol{F}^{(0)} = 6\pi\mu a(\boldsymbol{U}_a - \boldsymbol{0})$$

$$\boldsymbol{u}^{(0)}(\boldsymbol{x}) = \mathcal{J}(\boldsymbol{x} - \boldsymbol{x}_a) \cdot \boldsymbol{F}^{(0)}$$

place particle "b"

$$\boldsymbol{F}^{(1)} = 6\pi\mu a(\boldsymbol{U}_b - \boldsymbol{u}^{(0)}(\boldsymbol{x}_b))$$

$$\boldsymbol{u}^{(1)}(\boldsymbol{x}) = \mathcal{J}(\boldsymbol{x} - \boldsymbol{x}_b) \cdot \boldsymbol{F}^{(1)}$$

$$\mathbf{F}^{(2)} = 6\pi\mu a(\mathbf{U}_a - \mathbf{u}^{(1)}(\mathbf{x}_a))$$

$$\boldsymbol{u}^{(2)}(\boldsymbol{x}) = \mathcal{J}(\boldsymbol{x} - \boldsymbol{x}_a) \cdot \boldsymbol{F}^{(2)}$$

$$\boldsymbol{F}^{(3)} = 6\pi\mu a(\boldsymbol{U}_b - \boldsymbol{u}^{(2)}(\boldsymbol{x}_b))$$

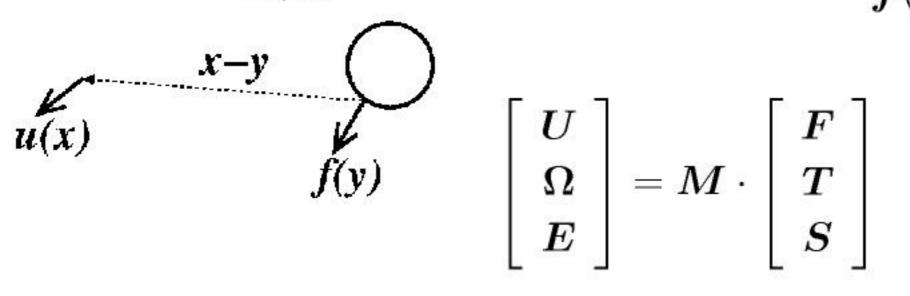
2. Boundary Value Problem

Integral equation

$$\boldsymbol{u}(\boldsymbol{x}) = -\frac{1}{8\pi\mu} \int dS(\boldsymbol{y}) \, J(\boldsymbol{x} - \boldsymbol{y}) \, \cdot \boldsymbol{f}(\boldsymbol{y})$$
 $\boldsymbol{u}(\boldsymbol{y}) \Rightarrow \boldsymbol{U}, \boldsymbol{\Omega}, \boldsymbol{E}$ $\boldsymbol{f}(\boldsymbol{y}) \Rightarrow \boldsymbol{F}, \boldsymbol{T}, \boldsymbol{S}$

Boundary condition

$$egin{array}{lll} m{u}(m{y}) & \Rightarrow & m{U}, m{X}, m{E} \ m{f}(m{y}) & \Rightarrow & m{F}, m{T}, m{S} \end{array}$$



$$egin{bmatrix} oldsymbol{U} \ oldsymbol{\Omega} \ oldsymbol{E} \end{bmatrix} = oldsymbol{M} \cdot egin{bmatrix} oldsymbol{F} \ oldsymbol{T} \ oldsymbol{S} \end{bmatrix}$$

Mobility problem

ex. sedimentation

Resistance problem

ex. porous medium

given : $\boldsymbol{F}, \boldsymbol{T}, \boldsymbol{E}$

unknown : U, Ω, S

given : $\boldsymbol{U}, \boldsymbol{\Omega}, \boldsymbol{E}$

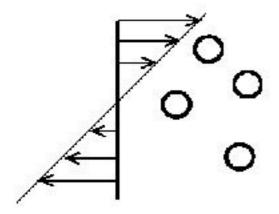
unknown : $\boldsymbol{F}, \boldsymbol{T}, \boldsymbol{S}$

2. Results

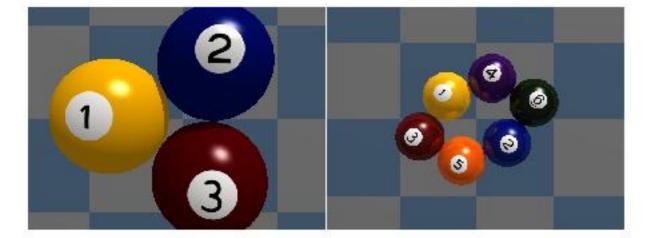
Shear flow

(force-free, torque-free)

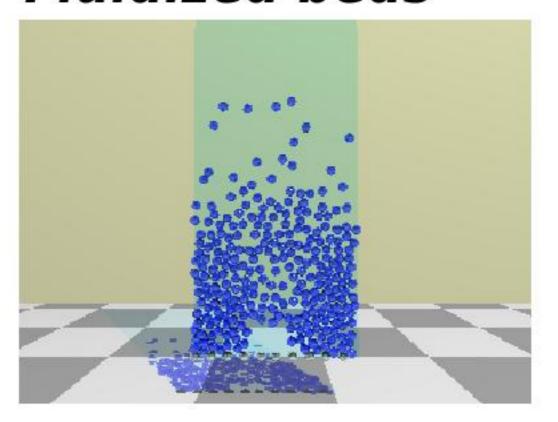
$$F = T = 0, \quad E \neq 0$$



$$\left[egin{array}{c} oldsymbol{U} \ oldsymbol{\Omega} \ oldsymbol{E} \end{array}
ight] = oldsymbol{M} \cdot \left[egin{array}{c} oldsymbol{0} \ oldsymbol{0} \ oldsymbol{S} \end{array}
ight]$$



Fluidized beds



3. Stokesian dynamics

[Brady, Bossis (1988) Annu.Rev.Fluid Mech.]

Multipole Expansion

$$u(x) = -\frac{1}{8\pi\mu} \sum_{\beta=1}^{N} \int_{S_{\beta}} dS(y) J(x-y) \cdot f(y)$$

$$egin{aligned} &= \sum_{eta=1}^N \mathcal{J}(oldsymbol{x}-oldsymbol{x}^eta) \cdot oldsymbol{F}^eta \ &+ \mathcal{R}(oldsymbol{x}-oldsymbol{x}^eta) \cdot oldsymbol{T}^eta \ &+ \mathcal{K}(oldsymbol{x}-oldsymbol{x}^eta) \cdot oldsymbol{S}^eta + \cdots \end{aligned}$$

$$\Rightarrow$$

$$\left[egin{array}{c} oldsymbol{U} \ oldsymbol{\Omega} \ oldsymbol{E} \ oldsymbol{U} \ dots \end{array}
ight] = \mathcal{M} \cdot \left[egin{array}{c} oldsymbol{F} \ oldsymbol{T} \ oldsymbol{S} \ oldsymbol{\mathcal{F}} \ dots \end{array}
ight]$$

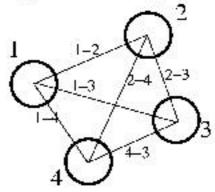
p: order of truncation

Lubrication

by 2-body EXACT solution

$$oldsymbol{L}^{ ext{2B}} := oldsymbol{R}^{ ext{2B}} - \left(oldsymbol{M}^{ ext{2B}}
ight)^{-1}$$

(short range)



$$\left[egin{array}{c} m{F} \ m{T} \ m{S} \end{array}
ight] = \left(m{M}^{-1} + m{L}
ight) \cdot \left[egin{array}{c} m{U} \ \Omega \ m{E} \end{array}
ight]$$

$$\left. \begin{array}{c} N=2\\ p\to \infty \end{array} \right\} \quad \Rightarrow \quad \text{recover EXACT solution}$$

3. Stokesian dynamics

Bottleneck?

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{U}$$

$$egin{array}{lcl} oldsymbol{U} & = & \left(oldsymbol{M}^{-1} + oldsymbol{L}
ight)^{-1} \cdot oldsymbol{F} \ & \iff & \\ \left(oldsymbol{I} + oldsymbol{M} \cdot oldsymbol{L}
ight) \cdot oldsymbol{U} & = & oldsymbol{M} \cdot oldsymbol{F} \end{array}$$

• inversion of matrix : $O(N^3)$

[KI (2002) J.Fluid Mech.]

Iterative Method

By CG-type iterative method

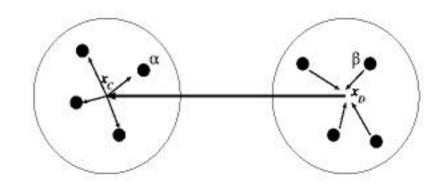
matrix-vector product : O(N²)

$$oldsymbol{U}' = oldsymbol{M} \cdot oldsymbol{F}'$$

Fast Multipole Method

[Greengard-Rokhlin (1987) J.Comp.Phys.]

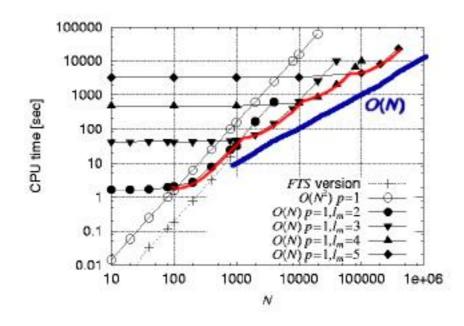
 \bullet O(N) for $U' = M \cdot F'$

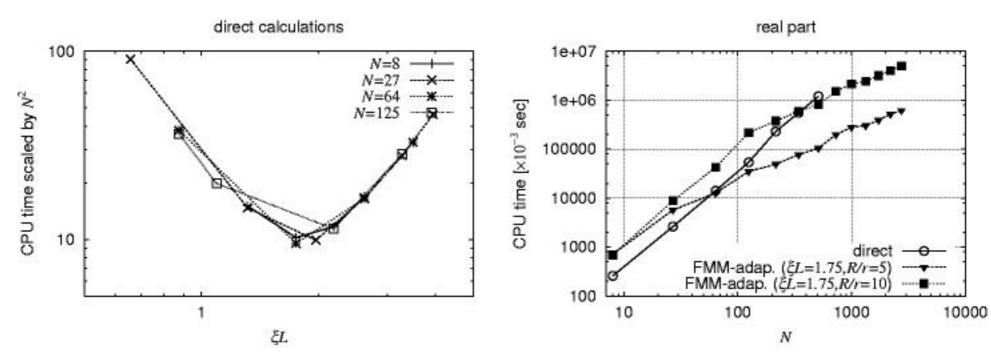


3. Results

[KI (2002) J.Fluid Mech.]

Improved?

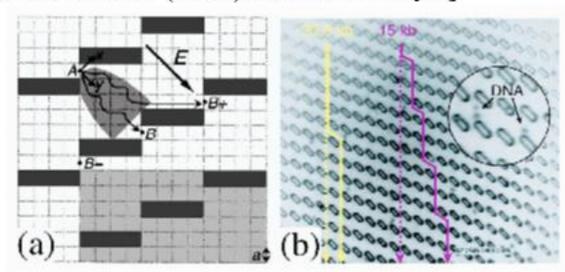




4. Nanotechnology

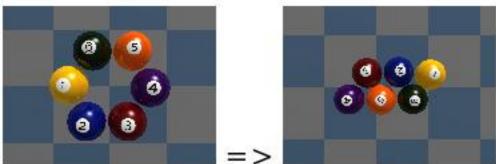
Experimental Results

[Squires, Quake (2005) Rev.Mod.Phys.]

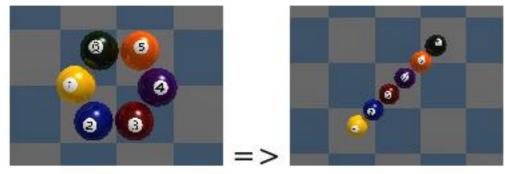


Simulation Results

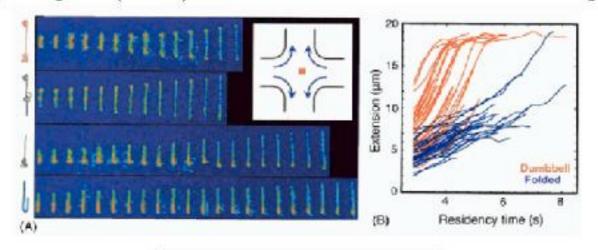
simple shear:

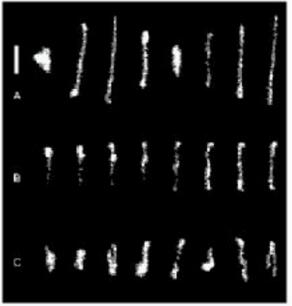


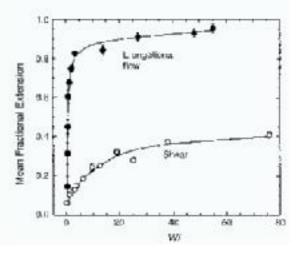
pure strain:



[Shaqfeh (2005) J.Non-Newtonian Fluid Mech.]







5. Acknowledgements

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