Microhydrodynamics

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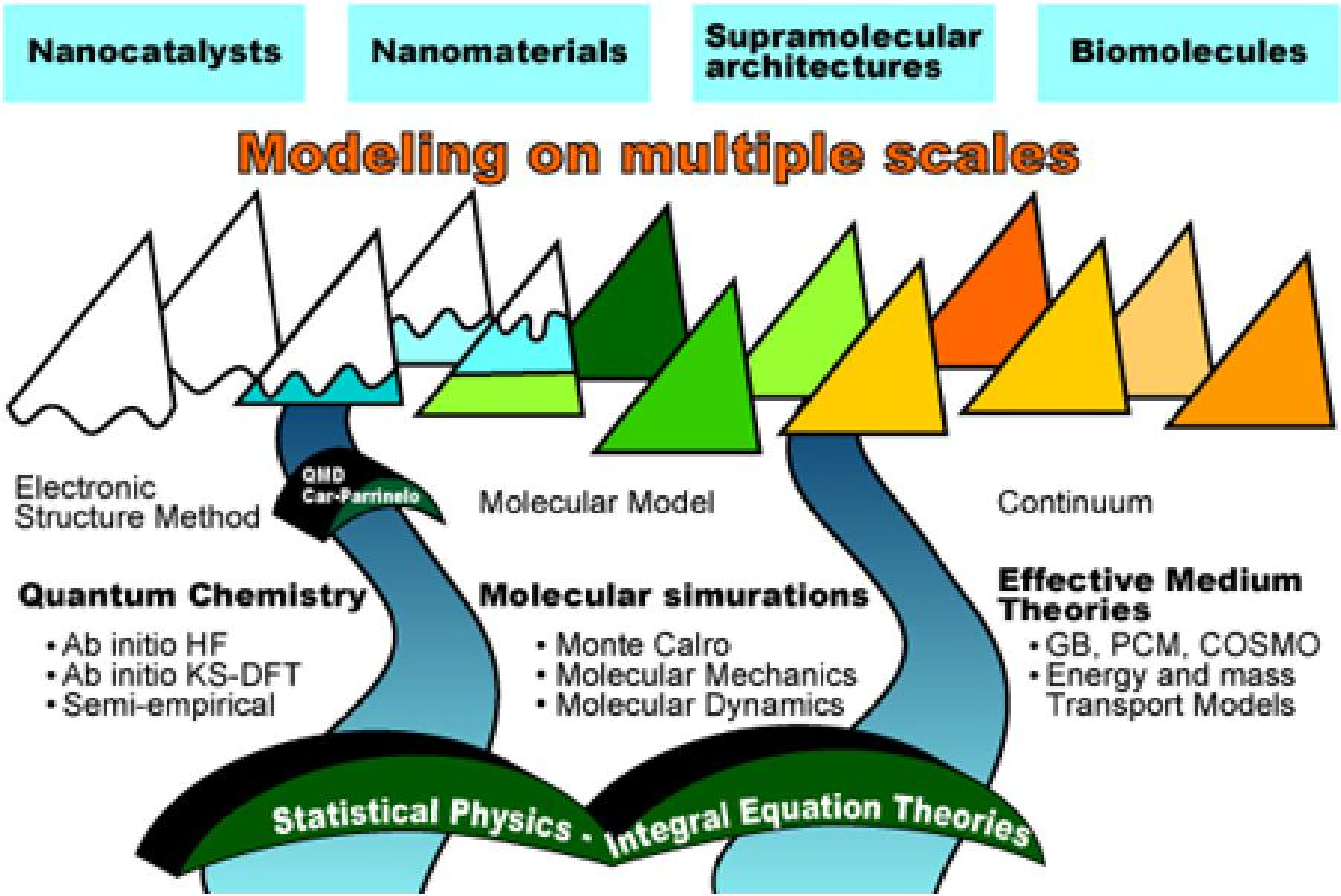
May 24, 2007

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

1. Multiple Scales



[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 : $Re = \dfrac{\rho L U}{\mu}$

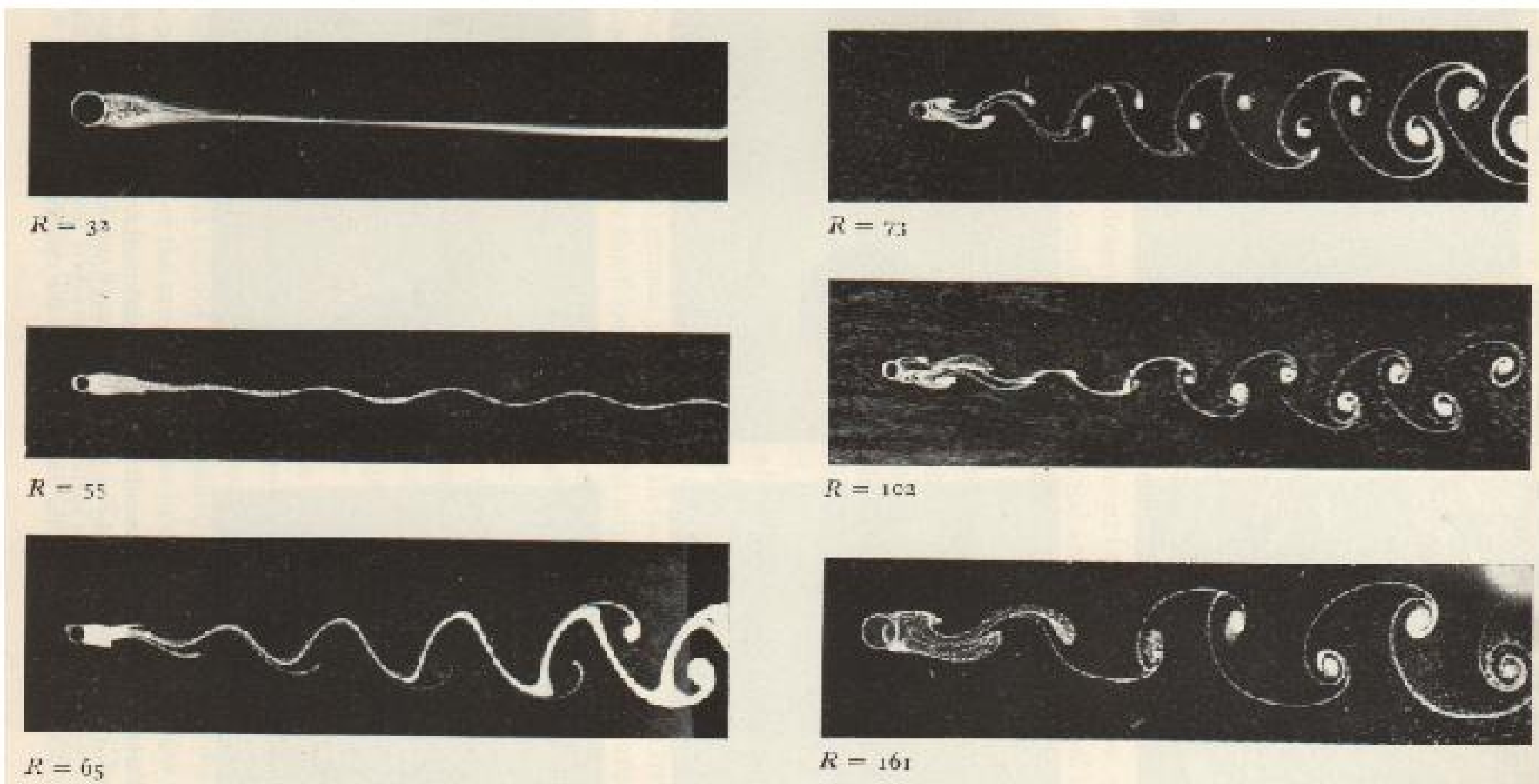


Figure 4.12.6. Streak lines in the wake behind a circular cylinder in a stream of oil. (From Homann 1936a.)

[Batchelor "An Introduction To Fluid Dynamics"]

1. Multi-Scale in Particle Systems

Atoms/Molecules

- Molecular dynamics

$$\boldsymbol{m} \cdot \frac{\mathrm{d}\boldsymbol{U}}{\mathrm{d}t} = \boldsymbol{F}$$

intermolecular,
electrostatic, ...
forces.

Dispersions

(colloids, polymers)

- Brownian dynamics
- Stokesian dynamics

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

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

$= -\boldsymbol{R} \cdot \boldsymbol{U}$

$\boldsymbol{F}^{\mathrm{B}}$: Brownian force

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

$\boldsymbol{F}^{\mathrm{ext}}$: external force

Gnarular systems

- Granular dynamics

Stars and Galaxy

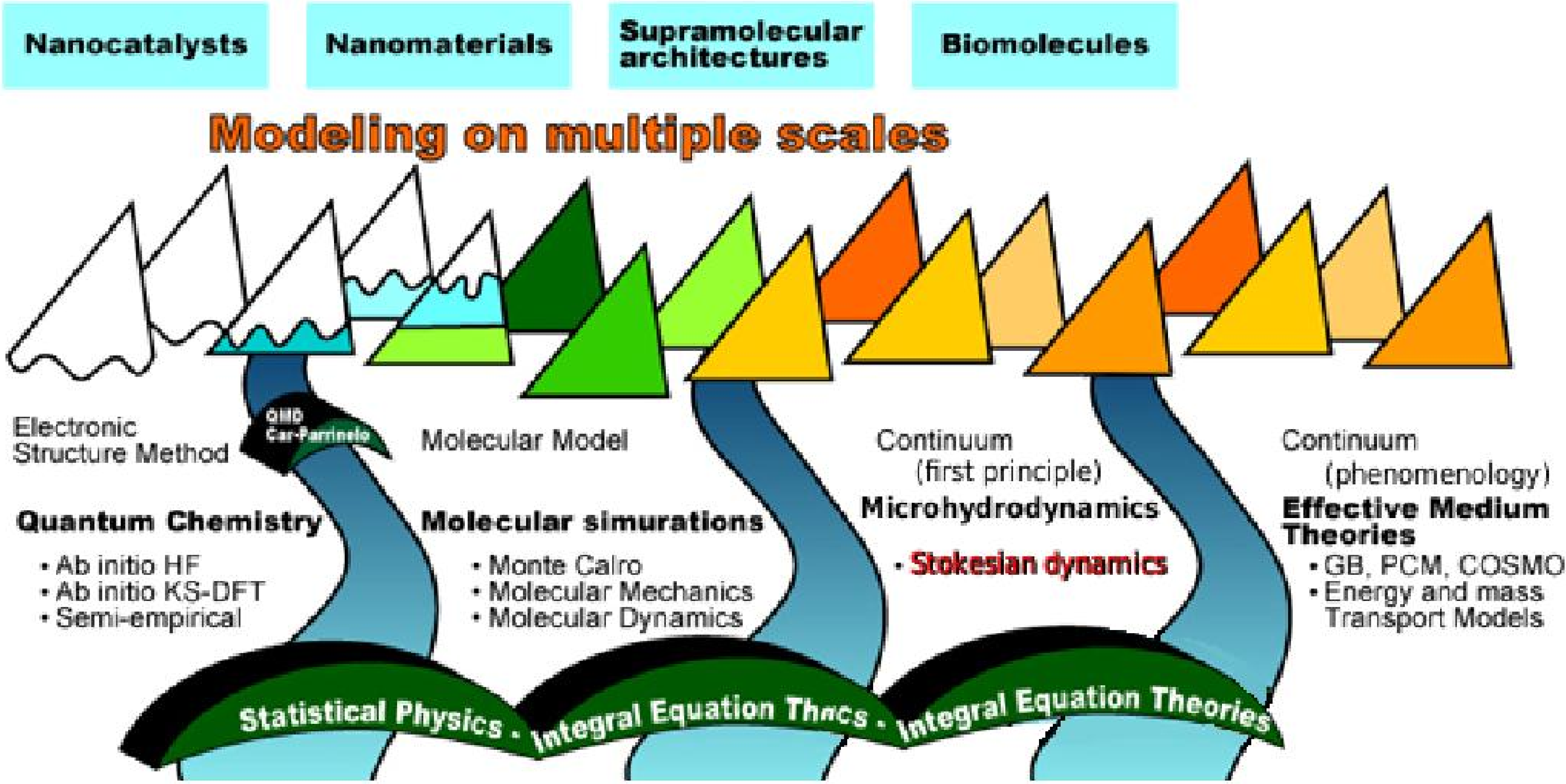
- Stellar dynamics

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.

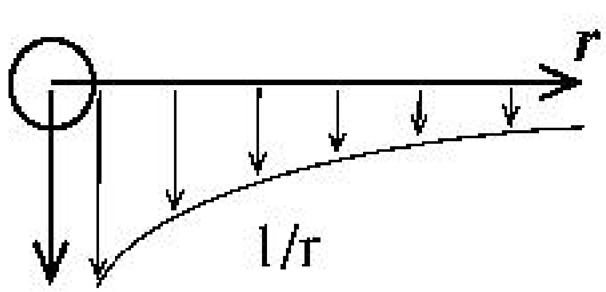
$$0 = -\boldsymbol{\nabla} p + \mu \nabla^2 \boldsymbol{u},$$

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

point force

$$\boldsymbol{u}(\boldsymbol{x}) = \frac{1}{8\pi\mu} \mathsf{J}(\boldsymbol{x} - \boldsymbol{x}_0) \cdot \boldsymbol{F}_0$$

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



Stokes drag

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

Electrostatics

Poisson eq.

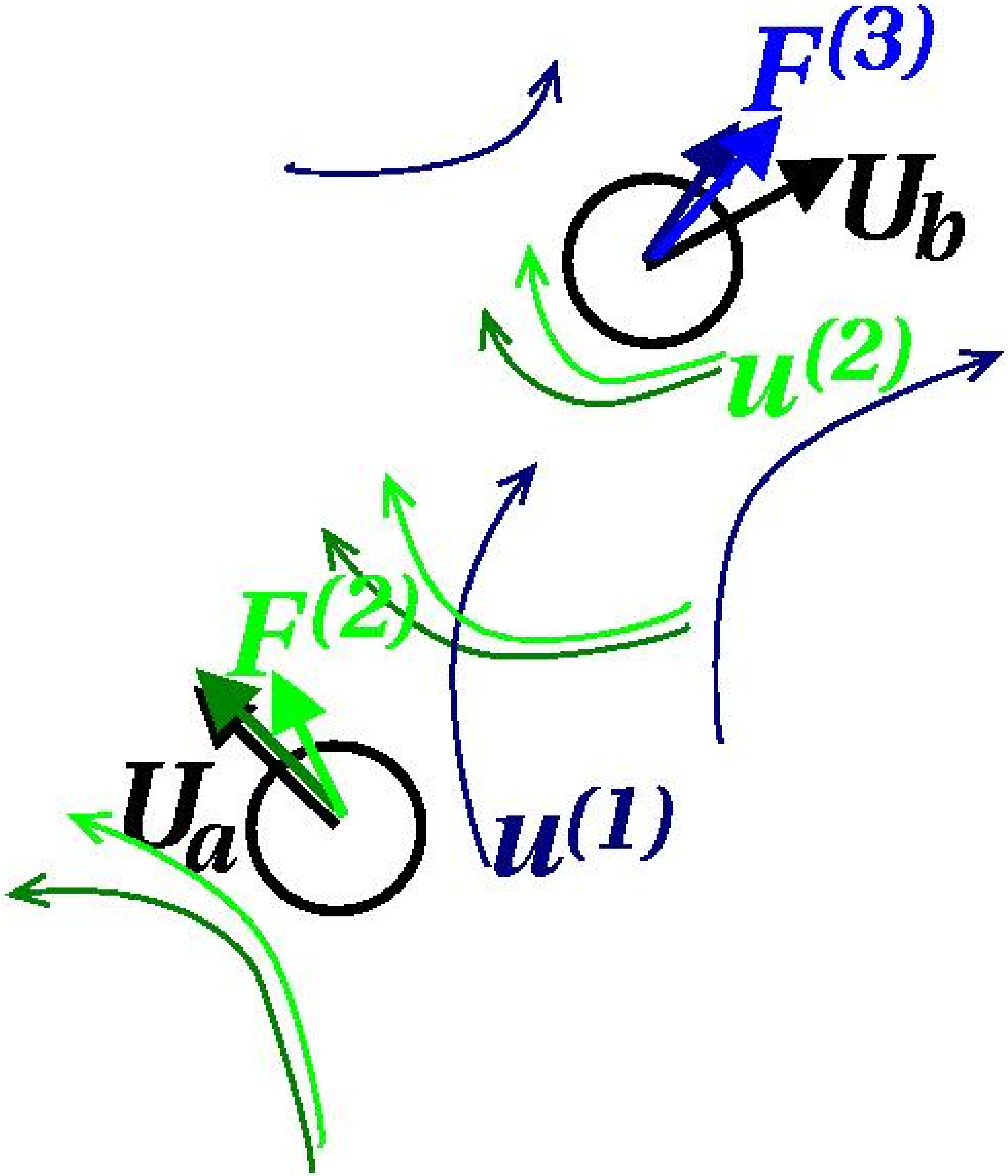
$$-\nabla^2 \phi = \frac{\rho}{\epsilon_0}$$

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"

$$F^{(0)} = 6\pi\mu a(U_a - 0)$$

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

place particle "b"

$$F^{(1)} = 6\pi\mu a(U_b - u^{(0)}(x_b))$$

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

$$F^{(2)} = 6\pi\mu a(U_a - u^{(1)}(x_a))$$

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

$$F^{(3)} = 6\pi\mu a(U_b - u^{(2)}(x_b))$$

2. Boundary Value Problem

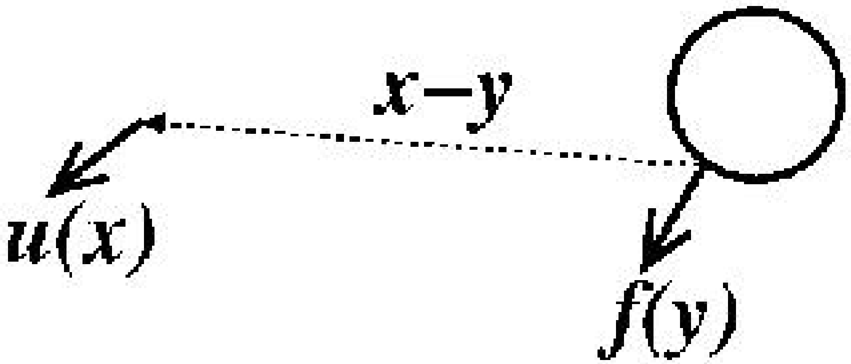
Integral equation

$$\boldsymbol{u}(\boldsymbol{x}) = -\frac{1}{8\pi\mu}\int dS(\boldsymbol{y})\ \mathsf{J}(\boldsymbol{x}-\boldsymbol{y})\ \cdot \boldsymbol{f}(\boldsymbol{y})$$

Boundary condition

$$\boldsymbol{u}(\boldsymbol{y}) \Rightarrow \boldsymbol{U}, \boldsymbol{\Omega}, \boldsymbol{E}$$

$$\boldsymbol{f}(\boldsymbol{y}) \Rightarrow \boldsymbol{F}, \boldsymbol{T}, \boldsymbol{S}$$



$$\begin{bmatrix} \boldsymbol{U} \\ \boldsymbol{\Omega} \\ \boldsymbol{E} \end{bmatrix} = \boldsymbol{M} \cdot \begin{bmatrix} \boldsymbol{F} \\ \boldsymbol{T} \\ \boldsymbol{S} \end{bmatrix}$$

Mobility problem

ex. sedimentation

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

unknown : $\boldsymbol{U}, \boldsymbol{\Omega}, \boldsymbol{S}$

Resistance problem

ex. porous medium

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

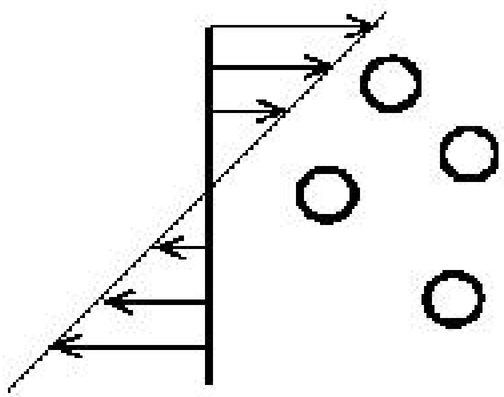
unknown : $\boldsymbol{F}, \boldsymbol{T}, \boldsymbol{S}$

2. Results

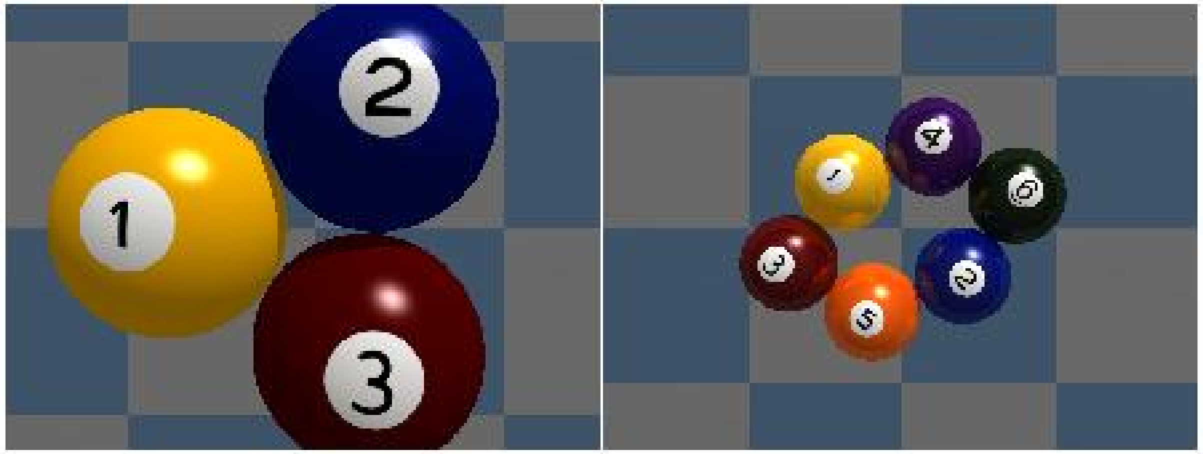
Shear flow

(force-free, torque-free)

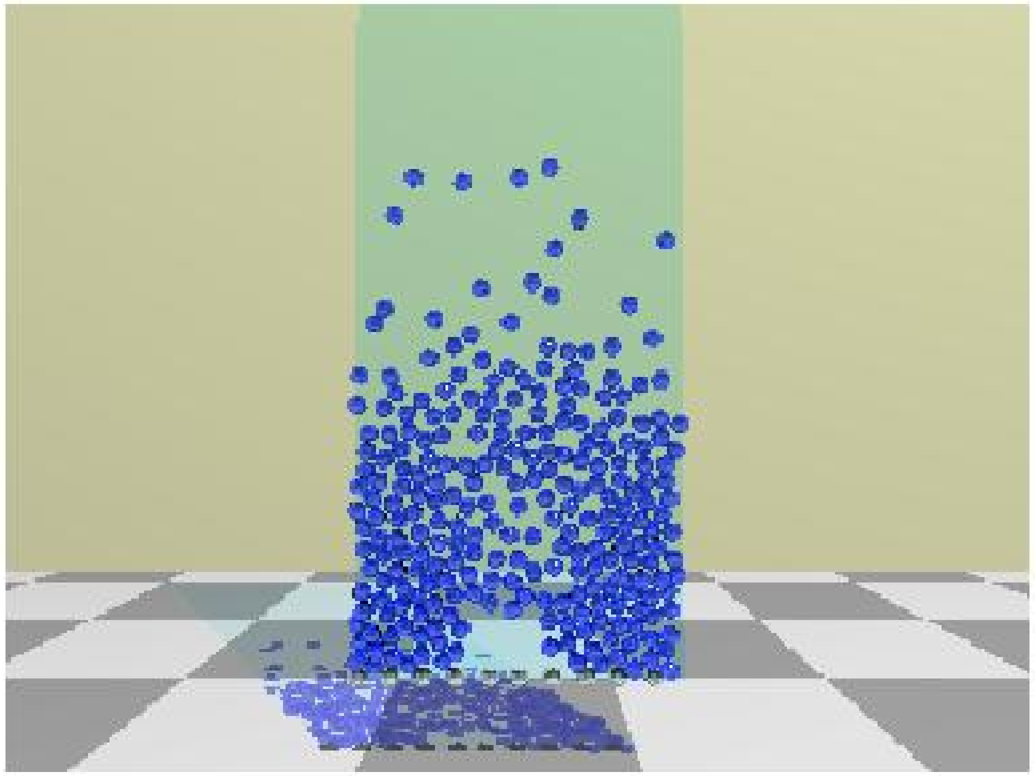
$$\boldsymbol{F} = \boldsymbol{T} = 0, \quad \boldsymbol{E} \neq 0$$



$$\begin{bmatrix} \boldsymbol{U} \\ \boldsymbol{\Omega} \\ \boldsymbol{E} \end{bmatrix} = \boldsymbol{M} \cdot \begin{bmatrix} 0 \\ 0 \\ \boldsymbol{S} \end{bmatrix}$$



Fluidized beds



3. Stokesian dynamics

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

Multipole Expansion

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

$$= \sum_{\beta=1}^{N}\mathcal{J}(x-x^\beta)\cdot F^\beta + \mathcal{R}(x-x^\beta)\cdot T^\beta + \mathcal{K}(x-x^\beta)\cdot S^\beta + \cdots$$

$\Rightarrow$

$$\begin{bmatrix} U \\ \Omega \\ E \\ \mathcal{U} \\ \vdots \end{bmatrix} = \mathcal{M}\cdot\begin{bmatrix} F \\ T \\ S \\ \mathcal{F} \\ \vdots \end{bmatrix}$$

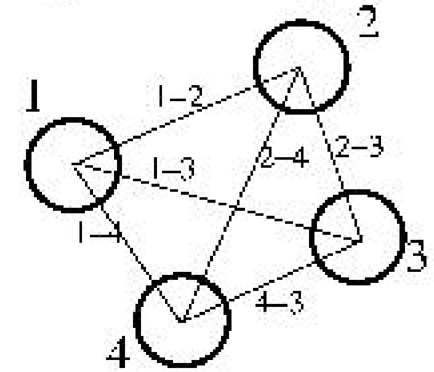
p : order of truncation

Lubrication

by 2-body EXACT solution

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

(short range)



$$\begin{bmatrix} F \\ T \\ S \end{bmatrix} = \left(M^{-1} + L\right)\cdot\begin{bmatrix} U \\ \Omega \\ E \end{bmatrix}$$

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

3. Stokesian dynamics

[KI (2002) J.Fluid Mech.]

Bottleneck?

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

$$\boldsymbol{U} = \left(\boldsymbol{M}^{-1} + \boldsymbol{L}\right)^{-1} \cdot \boldsymbol{F}$$

$$\Longleftrightarrow$$

$$\left(\boldsymbol{I} + \boldsymbol{M} \cdot \boldsymbol{L}\right) \cdot \boldsymbol{U} = \boldsymbol{M} \cdot \boldsymbol{F}$$

- inversion of matrix : $O(N^3)$

Iterative Method

By CG-type iterative method

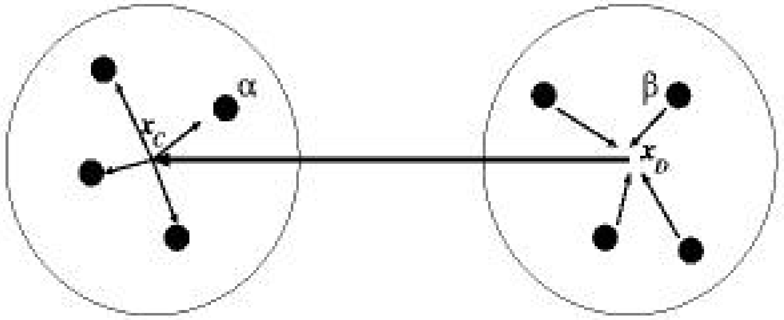
- matrix-vector product : $O(N^2)$

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

Fast Multipole Method

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

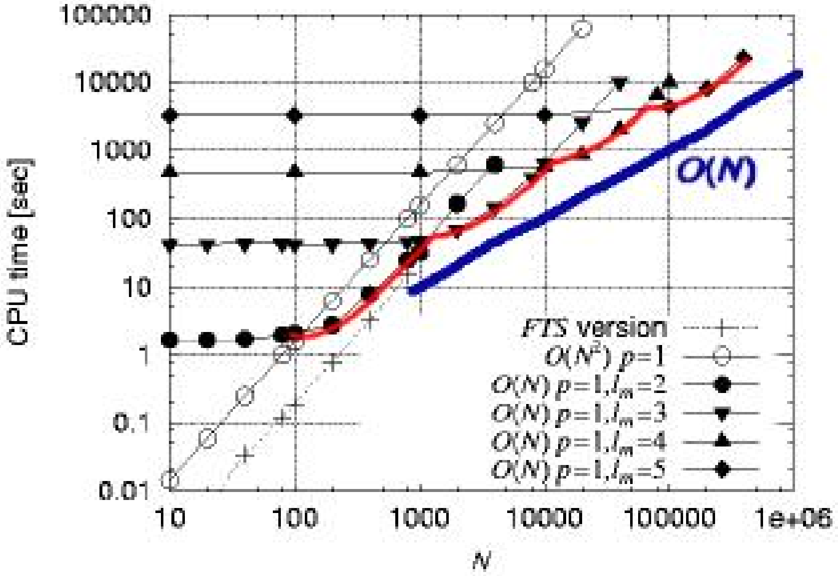
- $O(N)$ for $\boldsymbol{U}' = \boldsymbol{M} \cdot \boldsymbol{F}'$

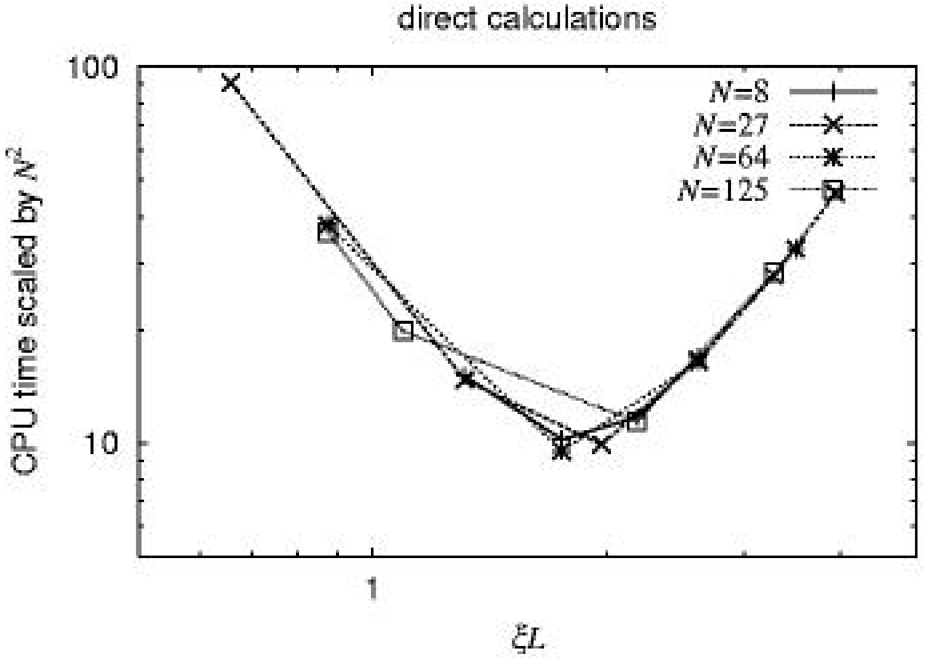


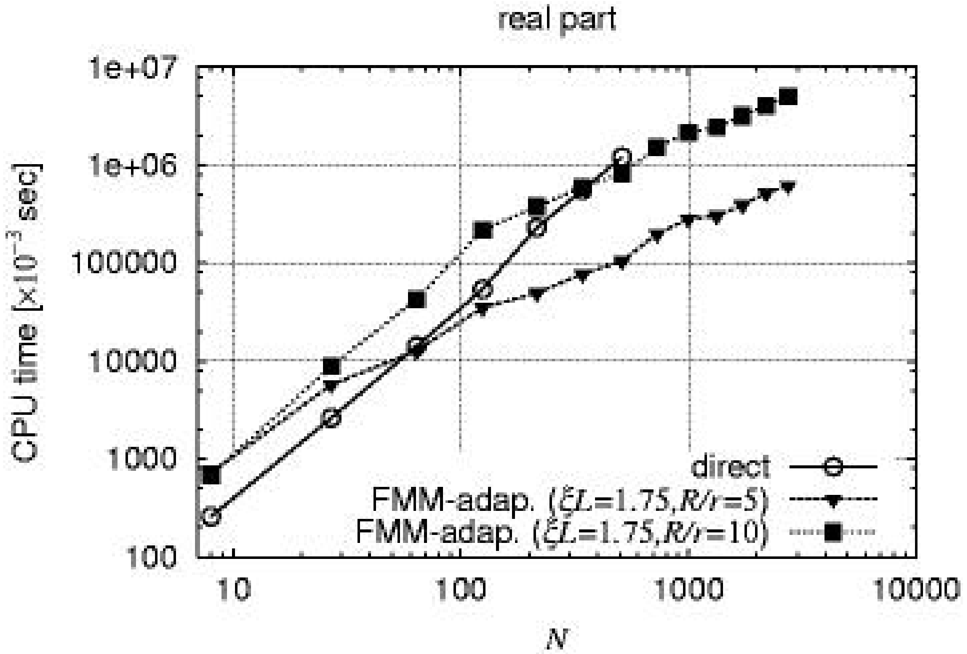
3. Results

[KI (2002) J.Fluid Mech.]

Improved?



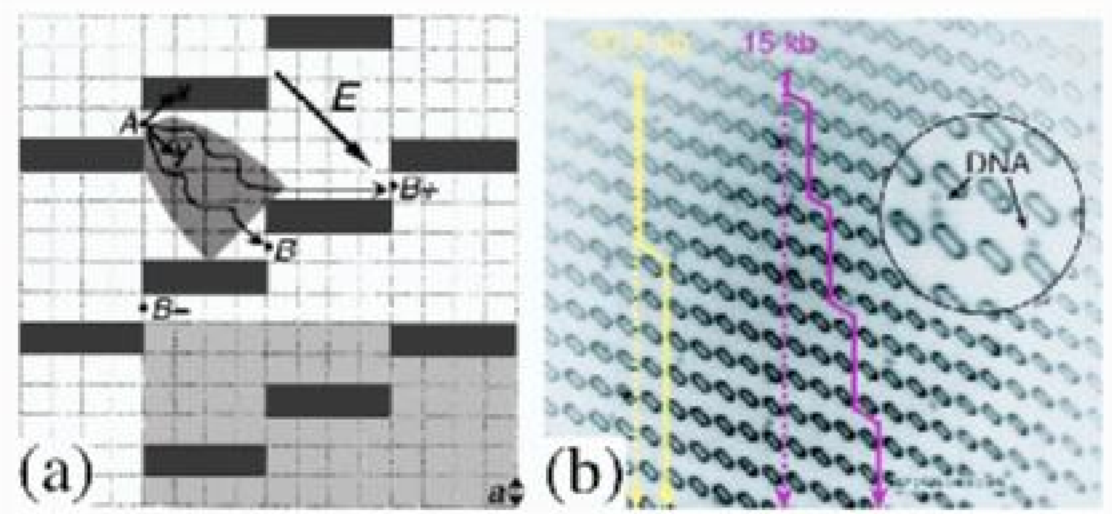




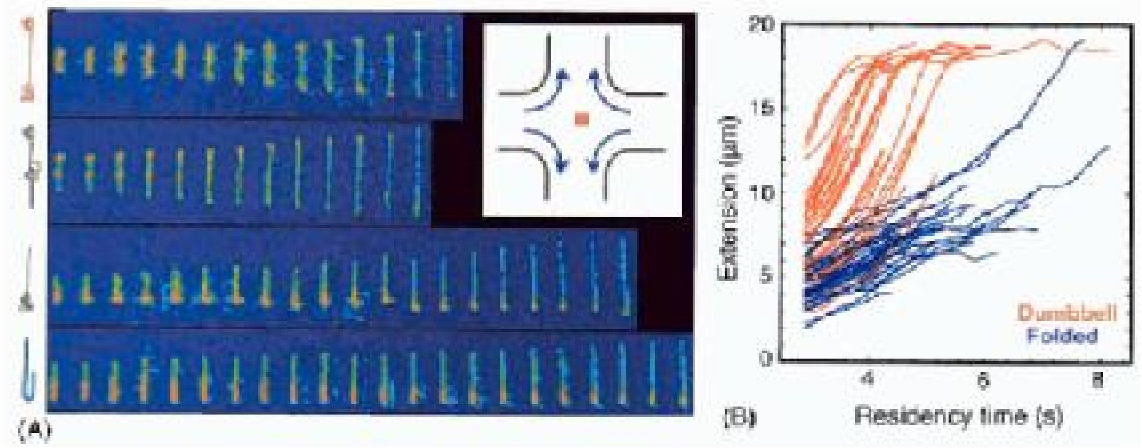
4. Nanotechnology

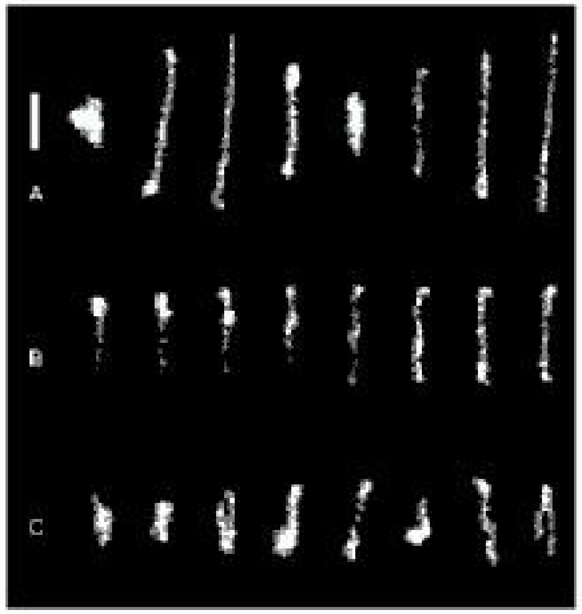
Experimental Results

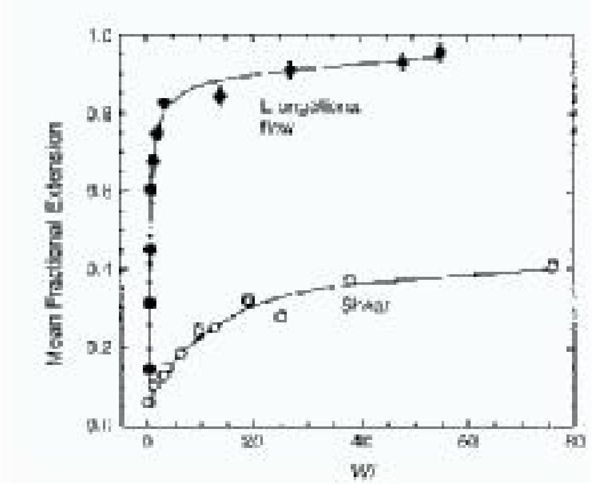
[Squires, Quake (2005) Rev.Mod.Phys.]



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

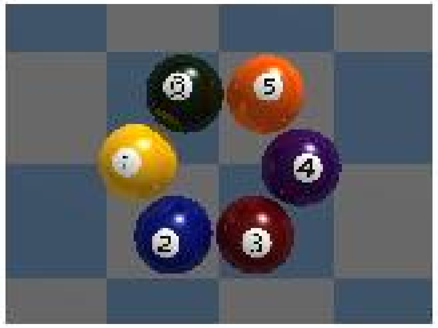






Simulation Results

simple shear:



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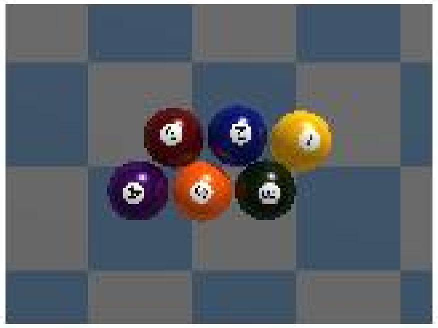
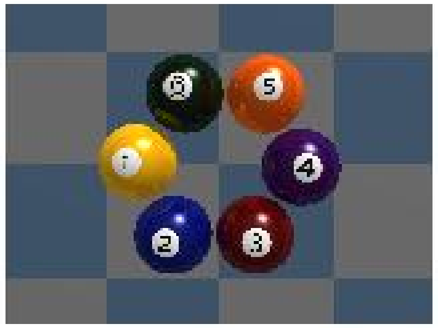


pure strain:



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5. Acknowledgements

- John F. Brady (Caltech)
- Masao Doi (U. Tokyo)
- Andrea Prosperetti (Johns Hopkins U.)
- David J. Jeffrey (U. Western Ontario)