Virtually every problem in applied math is a multiscale problem!

1. Boundary layer problems

$$\varepsilon \frac{\partial^2 u}{\partial x^2} + a(x)\frac{\partial u}{\partial x} = f(x)$$

2. Homogenization problems

$$-\nabla \cdot (a^\varepsilon(x)\nabla u^\varepsilon(x)) = f(x)$$

$$\text{e.g. } a^\varepsilon(x) = a\left(x, \frac{x}{\varepsilon}\right)$$

3. Fronts, vortex dynamics

$$\frac{\partial u}{\partial t} = \Delta u + \frac{1}{\varepsilon}\, u(1 - u^2)$$

Multiscale ideas are commonly used in numerical computations!

1. Multi-grid method

2. Adaptively mesh refinement

3. Fast multipole method

4. Domain decomposition

. . . . . .

So, **what is new?**

Multi-physics Modeling Hierarchy

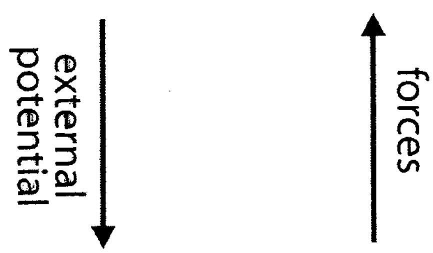
Gas, Plasmas	Liquids	Solids
Gas dynamics MHD	Hydrodynamics (Navier-Stokes)	Elasticity models Plasticity models
Kinetic theory	Density functional theory	Dislocation dynamics Phase-field models
	Brownian dynamics	Kinetic Monte Carlo
Particle simulation	Molecular dynamics	Molecular dynamics
		Electronic structures

Terminologies adopted here	Other terminologies
Serial coupling [6]	Pre-computing Microscopically-informed modeling Parameter passing
Concurrent coupling [6]	"On-the-fly" calculation [29] Solving equations without equations "Equation-free" [95]
Compression operator [55]	Projection operator [26] Restriction operator [95]
Reconstruction operator [106, 55] Reinitialization	Prolongation operator [26] Lifting operator [95]

Table 2. Comparison of the frequently used terminologies.

First principle-based molecular dynamics (FPMD)

Macroscale: Molecular Dynamics of atoms (nuclei)



microscale: Quantum mechanics of electrons

MD: $M_I \ddot{R}_I = -\nabla_{R_I} V_0(R_1, \cdots, R_N)$

Question: $V_0 = ?$

$$V_0 = \langle \Psi_0 | \hat{H}ee | \Psi_0 \rangle + \sum_{I,J} \frac{Z_i Z_j}{|R_I - R_J|}$$

$\Psi_0 = \Psi_0(r_1, r_2, \ldots, r_M) =$ ground state of electrons

$$\hat{H}ee = \sum -\frac{1}{2}\nabla_{r_i}^2 + \sum_{i<j} \frac{1}{|r_i - r_j|} + \sum_i v(r_i)$$

$$v(r_i) = -\sum_I \frac{Z_I}{|r_i - R_I|}$$

Car-Parrinello method

- Multi-physics
  (First principle based constitutive modeling)

- Multiple time scale
  (for nuclei and electrons)

- "On-the-fly" coupling

Missing: Spatial domain issues

Quasi-continuum Method

(Tadmor, Ortiz, Phillips 1996, A. Brandt 1992)

Given: Molecular mechanics model

$$E = \sum V_2(x_i, x_j) + V_3(x_i, x_j, x_k)$$

$$x_j = \text{position of } j\text{-th atom}$$

Goal: Compute macroscopic deformation of solid

Traditional approach: $u =$ displacement field

$$\min_u \int_\Omega W(\nabla u)\,dx$$

$$\begin{aligned} W &= \text{stored-energy density} \\ &= \text{ad hoc!} \end{aligned}$$

Quasicontinuum Method (Tadmor et. al 1996)

Microscopic model: $x_j = x_j^0 + u_j$

$$E = \sum V_2(x_i, x_j) + \sum V_3(x_i, x_j, x_k) + \dots$$

1. Selecting representative atoms $\{u_\alpha\}$

$$u_j = \sum_\alpha S_\alpha(x_j^0) u_\alpha$$

2. Summation rule

   Local: use Cauchy-Born rule

$$E \approx \sum_k |\Omega_k| \varepsilon(A_k), \quad A_k = \nabla u|_{\Omega_k}$$

   Nonlocal: summation over clusters

$$E \approx \sum_\alpha n_\alpha \varepsilon_\alpha(u_\alpha)$$

   Mixed: "Ghost force"

3. Adaptive mesh refinement

Limited to statics, zero temperature

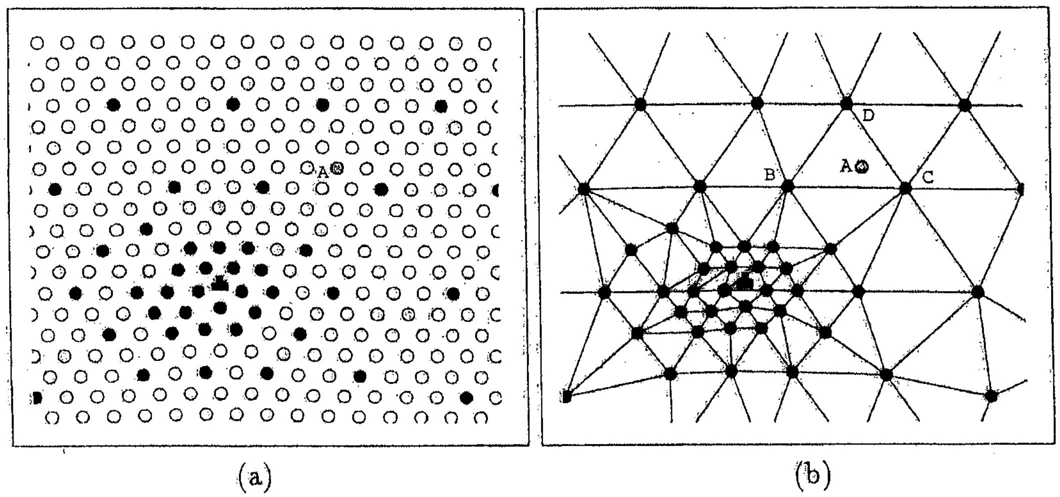
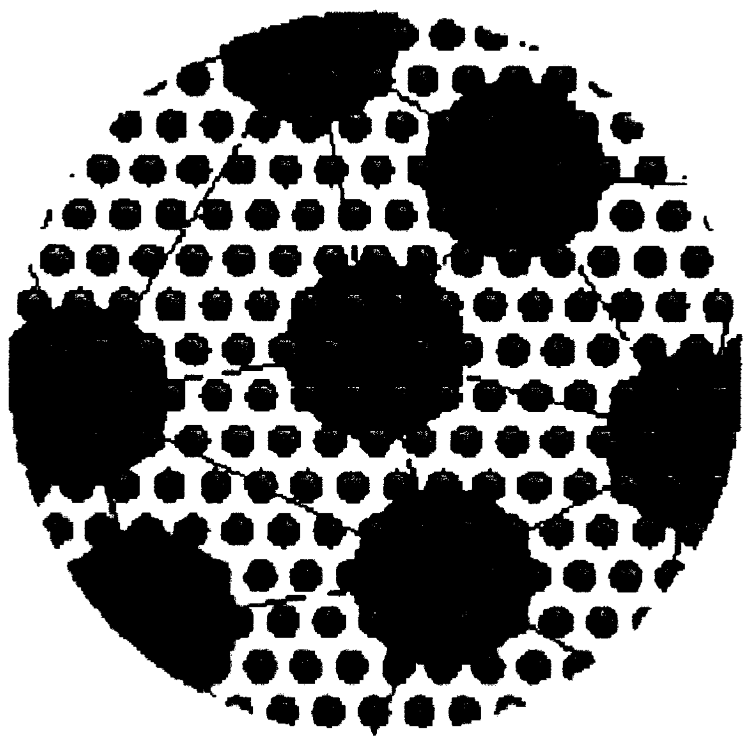


Figure 2: Selection of repatoms from all the atoms near a dislocation core are shown in (a), which are then meshed by linear triangular elements in (b). The density of the repatoms varies according to the severity of the variation in the deformation gradient.



Quasi-continuum method

Quasi-continuum

1. Reduction in DOF
   (Kinematics, no physics)

2. Localization of physical models:
   summation rule

Quasi-continuum

Successful for statics, $T = 0$

Issue of ghost force still remains

Key questions:

(1) Dynamics
(2) $T > 0$

Computing stress from atomistics

(1) solids, $T = 0$, $\sigma = \sigma(A)$

(2) solids, $T > 0$, $\sigma = \sigma(A, T)$

(3) solids, $\nabla T \neq 0$ $\sigma = \sigma(H, T, \nabla T)$

$q = q(A, T, \nabla T)$

(4) fluids, $\sigma = \sigma(A_t) = \sigma(D)$

$$
\begin{aligned}
u &= \text{displacement}, \\
A &= \nabla u = \text{deformation gradient} \\
v &= u_t = \text{velocity} \\
D &= \frac{1}{2}(\nabla v + \nabla v^T) = \text{rate of strain}
\end{aligned}
$$

Atomistic expression of stress for solids

$$\sigma = \frac{1}{|\Omega_0|} \sum_{i,j} f_{ij} \otimes (x_i^0 - x_j^0) c_{ij}$$

$f_{ij} =$ force between i-th and j-th atom

$x_i^0 =$ position of i-th atom in underformed configuration

$c_{ij} =$ proportion of segment $\overline{x_i^0 x_j^0}$ in Ω_0

$T = 0:$ $\quad \sigma = \nabla_A W_{CB}(A)$

$= $ Piola-Kirchhoff stress

$T > 0:$ "entropic contribution"

Connection of macro and micro models

Conservation of momentum (MD):

$$m(x,t) = \left\langle \sum_i p_i(t)\delta(q_i(t)-x) \right\rangle$$

$$\begin{cases} m_t + \nabla \cdot \tau = 0 \\ \tau(x,t) = \left\langle \sum_i \frac{1}{m_i}(p_i \otimes p_i)\delta(q_i - x) \right\rangle \\ \qquad + \left\langle \frac{1}{2}\sum_{j \neq i} \big((q_i - q_j) \otimes F_{ij}\big) \int_0^1 \delta\big(\lambda q_i + (1-\lambda)q_j - x\big) d\lambda \right\rangle \end{cases}$$

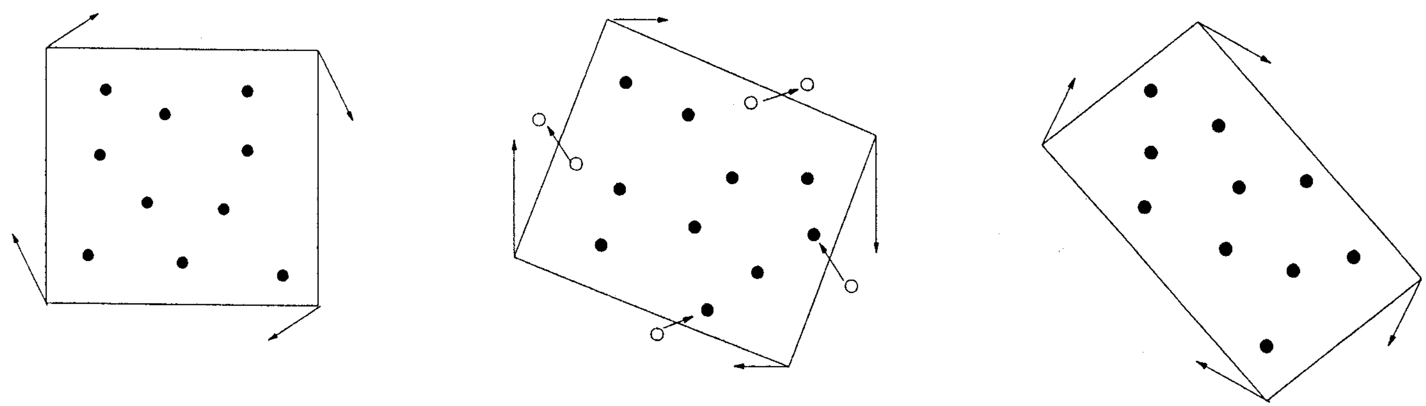
Irving-Kirkwood (1950)

The I-K formula (MD) needs to be localized !

Constant rate of strain MD

$$\nabla u = A = \begin{pmatrix} a & b & 0 \\ c & -a & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

a ,*b* and *c* are given by macro velocity field



- *Deforming the simulation box* $\frac{dX_i}{dt} = AX_i$
- *Periodic BC on the dynamically changing box*
- *Reinitialization*

Extracting the stresses using *I-K* formula

$$\tau(x,t)=\sum_i \frac{1}{m_i}(p_i\otimes p_i)\delta(q_i-x)+\frac{1}{2}\sum_{j\neq i}\left((q_i-q_j)\otimes F_{ij}\right)\int_0^1 \delta\left(\lambda q_i+(1-\lambda)q_j-x\right)d\lambda$$

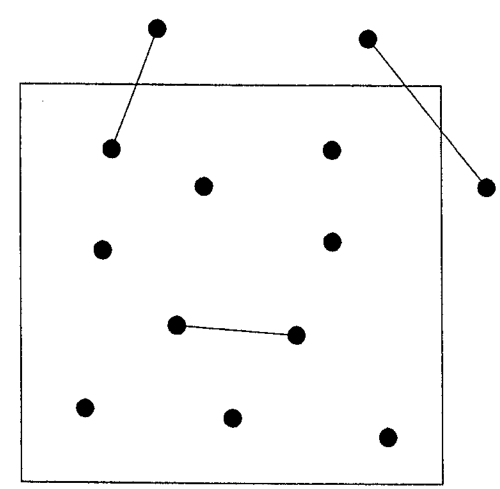
Average the momentum flux over space and time:

- $$\tau_L(t)=\frac{1}{|\Omega|}\sum_{q_i\in\Omega(t)}\frac{1}{m_i}(p_i\otimes p_i)+\frac{1}{2|\Omega|}\sum_{j\neq i}d_{ij}(q_i-q_j)\otimes F_{ij}$$

Ω : Area of the simulation box

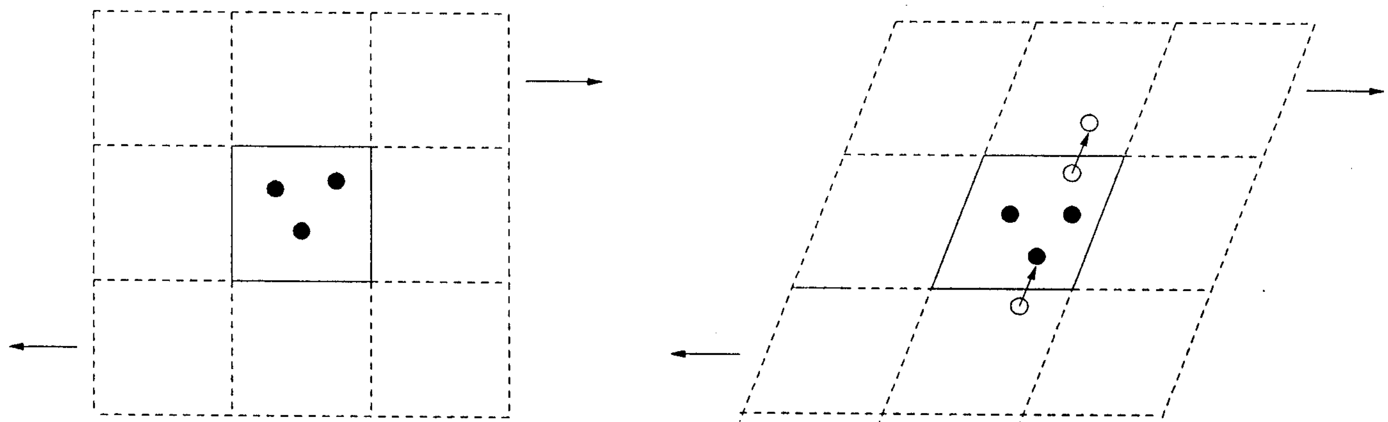
$$d_{ij}=\begin{cases}1, & \text{if } q_i,q_j\in\Omega\\ 0, & \text{if } q_i,q_j\in\Omega\\ c, & \text{if only one } q_i,q_j \text{ in } \Omega\end{cases}$$

- $$\tau_L=\frac{1}{T-T_0}\int_{T_0}^{T}\tau(t)dt$$



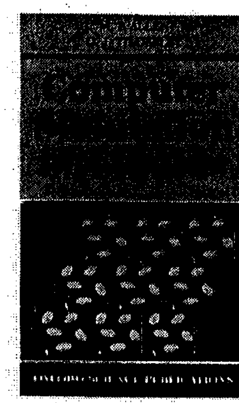
Constant rate of strain MD in 1D (pure shear)

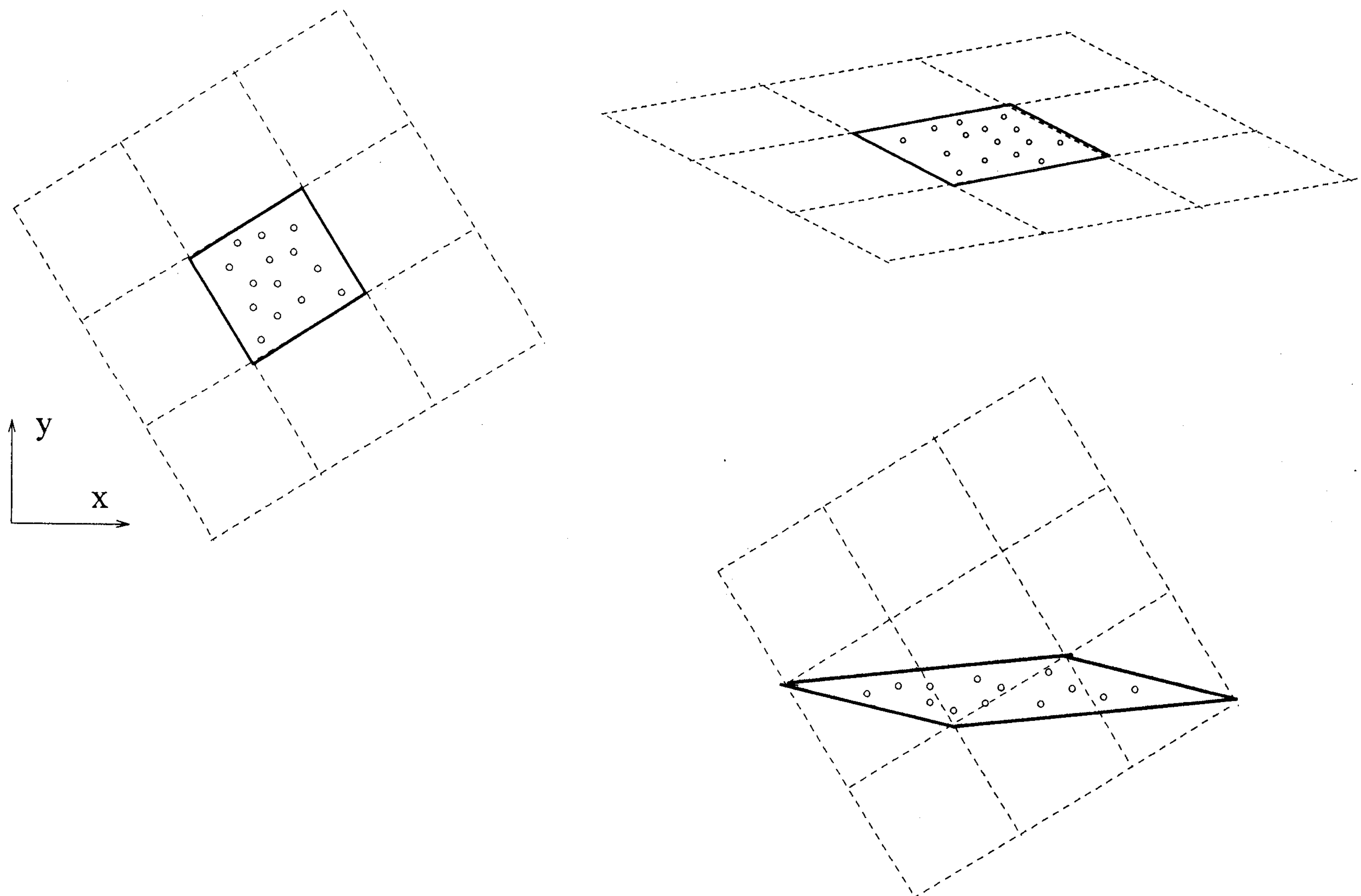
$$u(x,y) = by, \quad v(x,y) = 0, \quad w(x,y) = 0$$



Lees-Edwards BC (1972)

SLLOD algorithm (Hoover, Ladd)

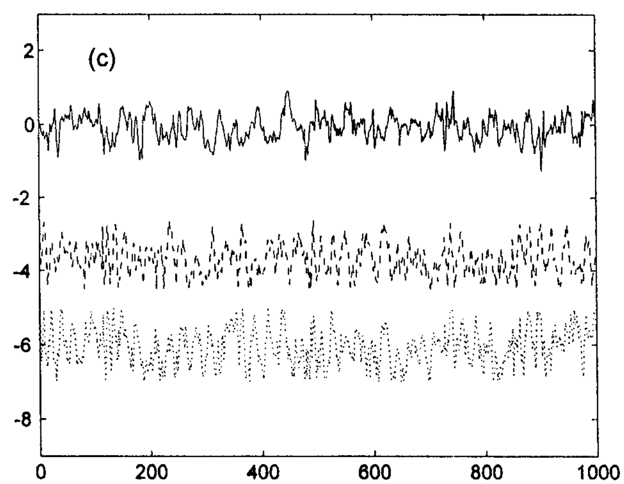


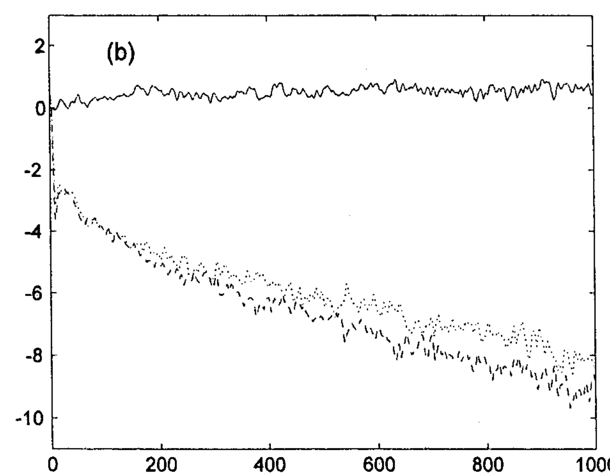

y
x

Example of stresses: Simple LJ fluids

$$\begin{cases} u = 0.18x \\ v = -0.18y \\ w = 0 \end{cases}$$

$$\begin{cases} u = 0.18y \\ v = w = 0 \end{cases}$$ without thermostat



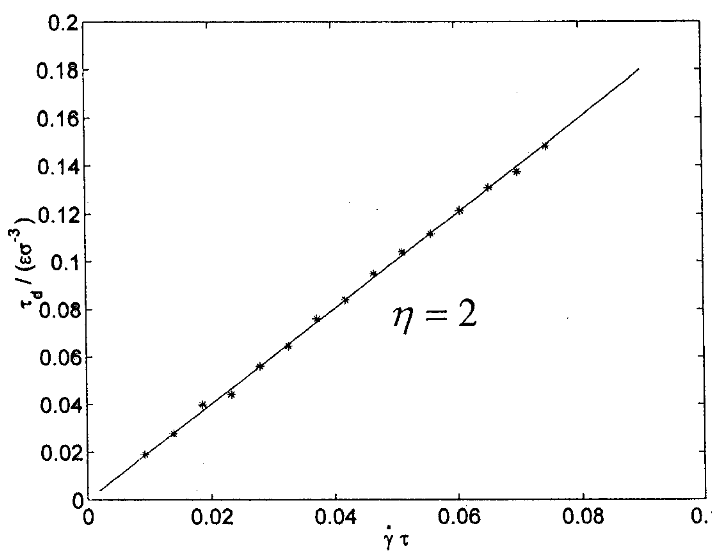


Example of stresses: Simple LJ fluids

$$\tau_d = \eta\dot{\gamma}$$

η : viscosity

$\dot{\gamma}$: shear rate

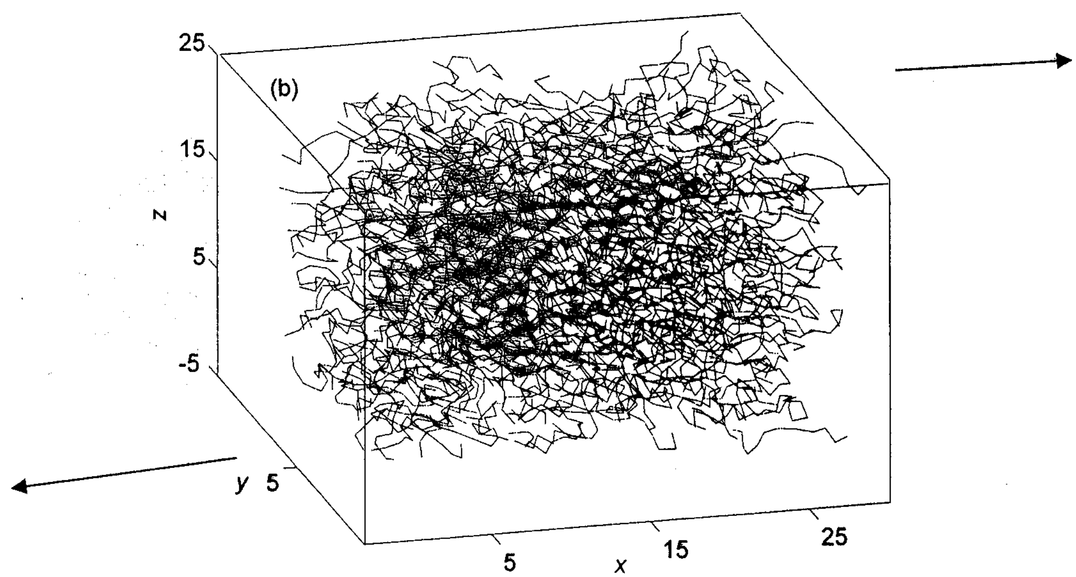


$\rho = 0.81\sigma^{-3}$, $T = 1.4\varepsilon / k_B$

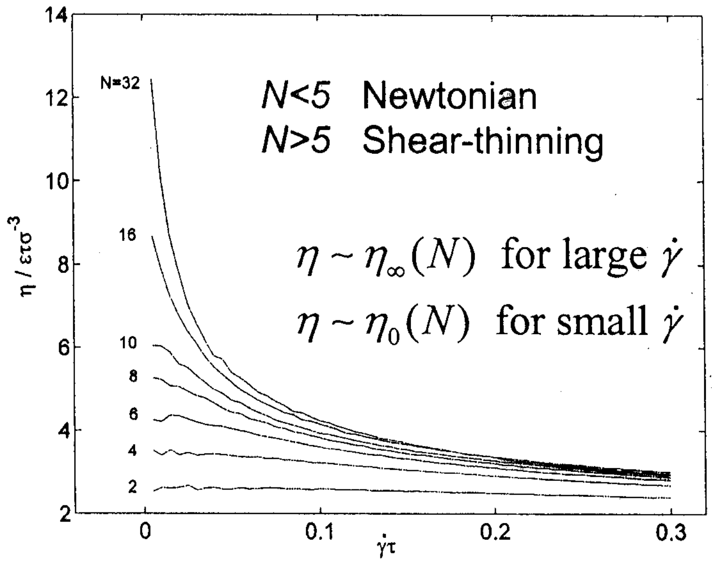
P. A. Thompson, M. O. Robbins, Phys. Rev. Lett. ***63****, 766(1989)*

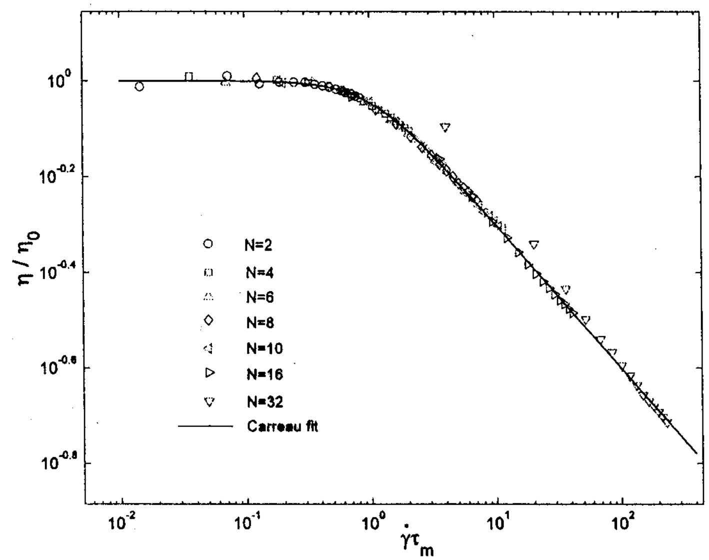
Study of the constitutive relation for polymeric fluids

$$u = \dot{\gamma} z, \; v = w = 0$$



Shear viscosity vs. Shear rate :





The data for short chains are well fitted by *Carreau function* :

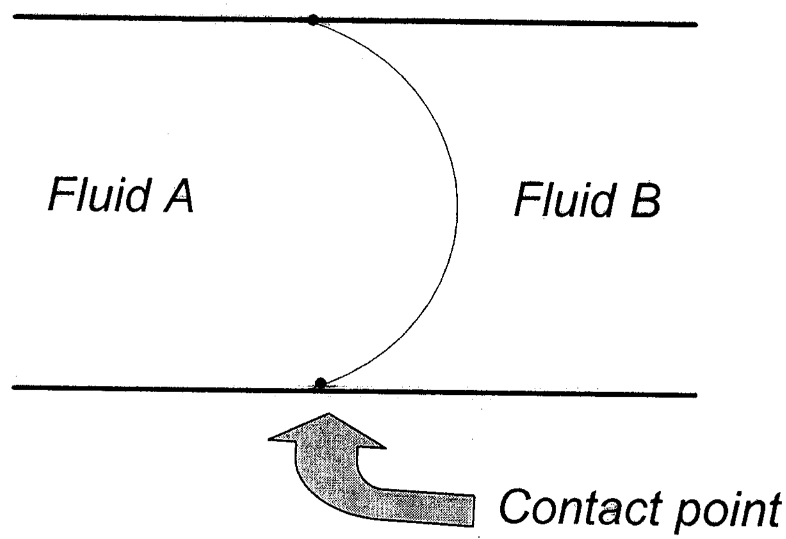
$$\eta = \eta_0 (1 + (\dot\gamma \tau_m)^2)^{(n-1)/2} \quad , \; n = 0.7$$

$\eta_0(N)$: zero-shear viscosity

$\tau_m(N)$: maximum relaxation time

Other example of shear-thinning fluids: ketchup, paint, blood ...

Example of multiscale method: Contact line dynamics

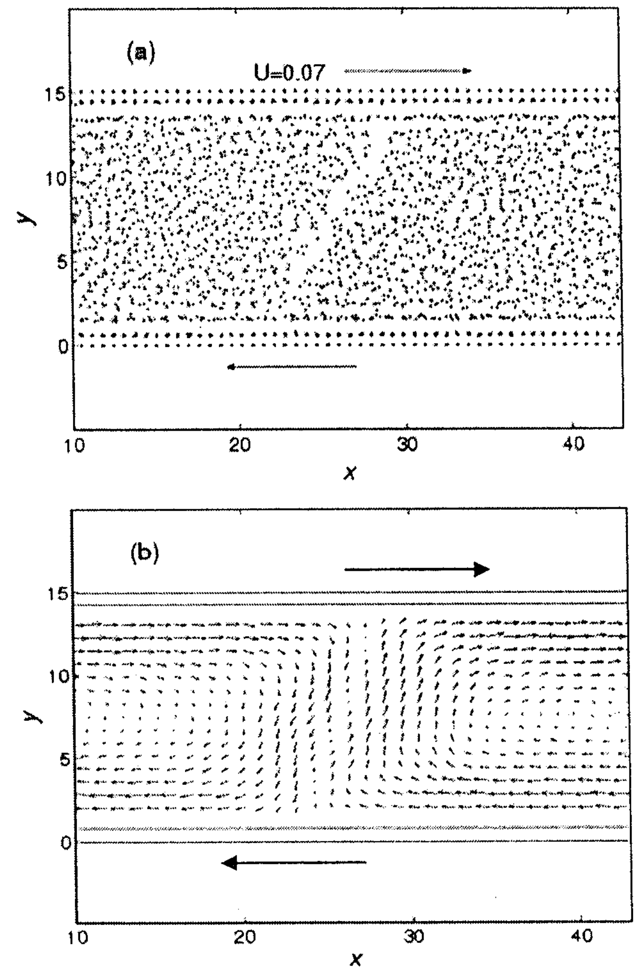


No-slip boundary condition is invalid near the contact line.

Direct MD simulation of Couette flow

$$V^{LJ}(r) = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \delta\left(\frac{\sigma}{r}\right)^{6}\right)$$

$$\delta = \begin{cases} -1 & \text{between Fluid } A \text{ and } B \\ +1 & \text{otherwise} \end{cases}$$



Example of Slip models:

Navier BC

Generalized Navier BC
(Qian, Wang, Sheng)

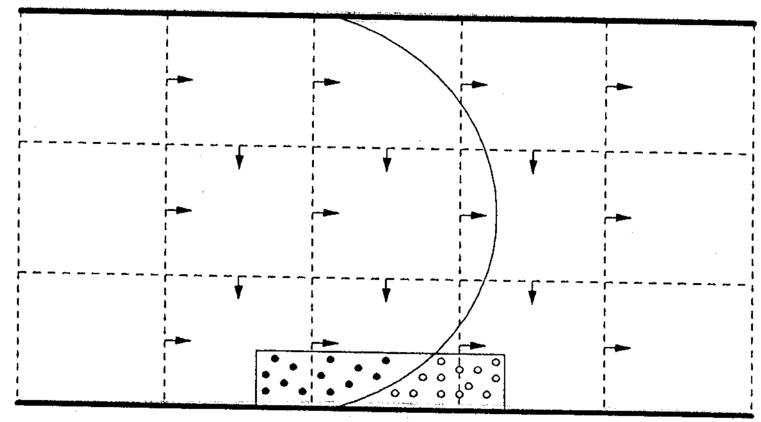
Flat precursor film model

van der Waals precursor film model

Greenspan slip model

Multiscale modeling of contact line dynamics

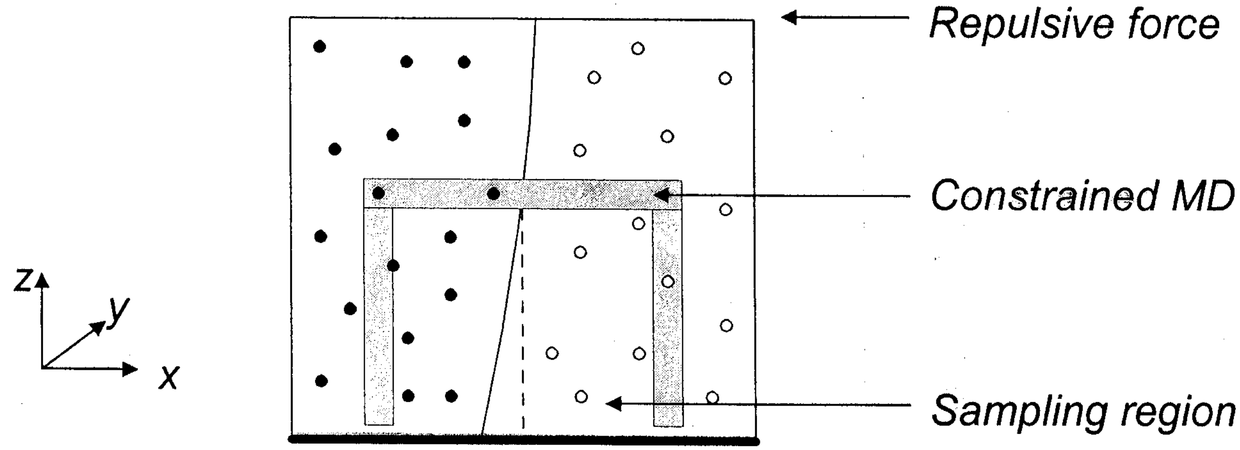
$$\begin{cases} \rho u_t + \nabla \cdot \tau = 0 \\ \nabla \cdot u = 0 \\ \dot{x}_\Gamma = u \end{cases}$$



$$\tau = \rho u \otimes u + pI - \mu(\nabla u + \nabla u^{\mathrm{T}}) + \gamma(I - \hat{n} \otimes \hat{n})\delta_\Gamma - f_0 x I$$

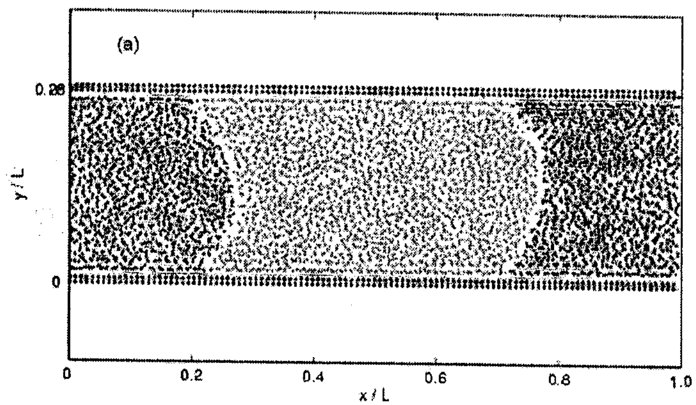
- Spatial discretization on staggered grid; The interface is represented by discrete points
- Surface tension is smoothed out to the neighboring points (*Peskin*)
- ***Tangential stress*** near the CL & ***Contact angle*** are calculated from *MD*

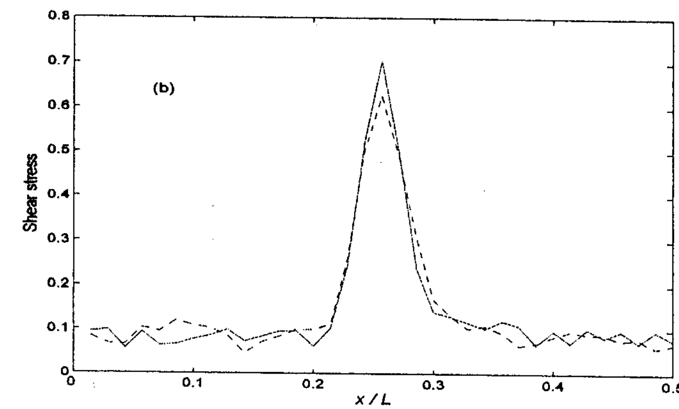
Multiscale modeling of contact line dynamics

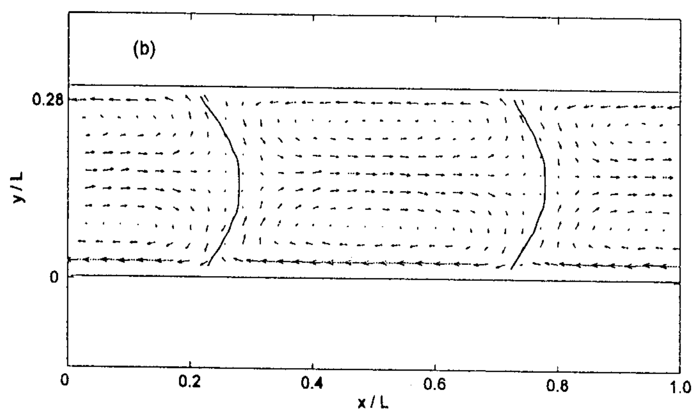


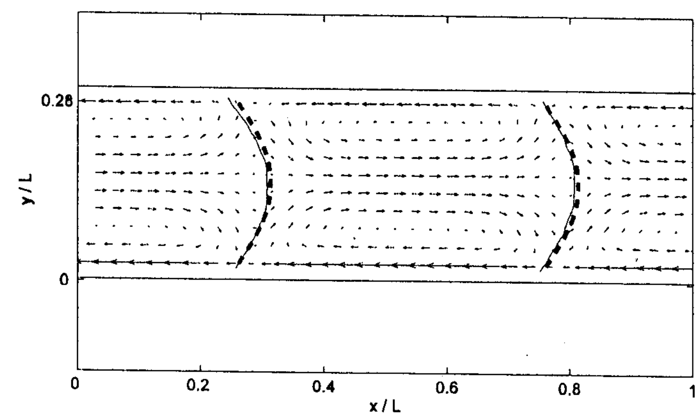
- Periodic in *y*;
- Particle species needs to be changed when crossing the boundary in x direction
- The constraints in horizontal and vertical strips are imposed alternatively

Validation of the multiscale method









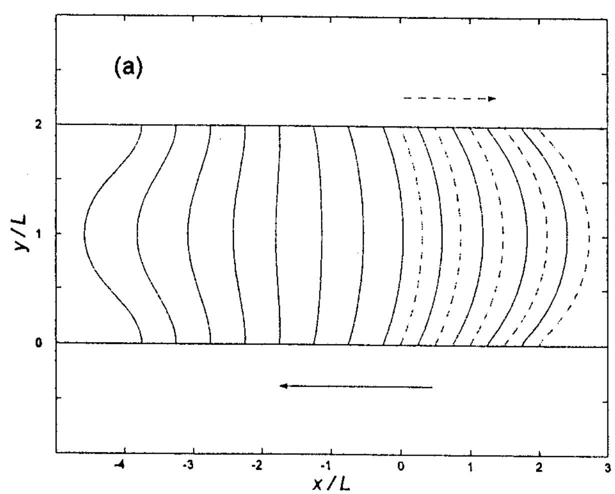
system size: $69.7 \times 22.5 \times 5.16\ \sigma^3$;

ρ=0.81 ; η=2.0; γ=3.7

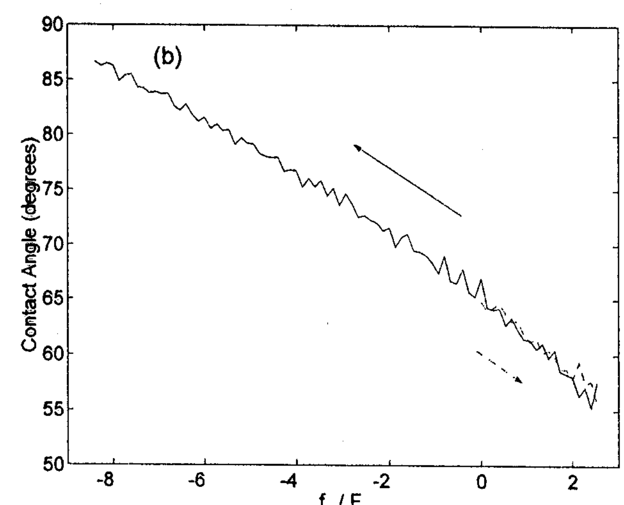
Application to a larger system : Asymmetric fluid-solid interaction

External force $f = f(t)$

Dynamics of interface



Dynamics of contact angle



system size : $1500\sigma \times 500\sigma$; ρ=0.81; μ=2.0; γ=3.7

Summary:
Issues in Multiscale Modeling

Conceptual: Multi-physics

Technical: How do we localize

- Domain decomposition
- Adaptive model refinement
- Equation-free (Kevrekidis, et.al)
- Heterogeneous multiscale method (HMM)

Key: Boundary condition

Mathematical: Understand transition between multi-physics models