\[
(\zeta n - 1)n \frac{\partial}{\partial t} + n \nabla = \frac{\mathcal{H}}{n_0}
\]

3. Fronts, vortex dynamics

\[
\left(\frac{\partial}{\partial t}, x\right) \nabla = (x) \nabla \cdot \mathbf{\varepsilon}
\]

\[
(x)f = ((x) \nabla \Delta (x) \nabla) \cdot \Delta
\]

2. Homogenization problems

\[
(x)f = \frac{x \theta}{n \varepsilon} (x) \nabla + \frac{\zeta x \theta}{n \varepsilon}
\]

1. Boundary layer problems

multiscale problem!

Virtually every problem in applied math is a
So, what is new?

1. Multi-grid method
2. Adaptively mesh refinement
3. Fast multipole method
4. Domain decomposition

Numerical computational multiscale ideas are commonly used in
## Multi-physics Modeling Hierarchy

<table>
<thead>
<tr>
<th>Gas, Plasmas</th>
<th>Liquids</th>
<th>Solids</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas dynamics</td>
<td>Hydrodynamics (Navier-Stokes)</td>
<td>Elasticity models</td>
</tr>
<tr>
<td>MHD</td>
<td></td>
<td>Plasticity models</td>
</tr>
<tr>
<td>Kinetic</td>
<td>Density functional theory</td>
<td>Dislocation dynamics</td>
</tr>
<tr>
<td>theory</td>
<td></td>
<td>Phase-field models</td>
</tr>
<tr>
<td></td>
<td>Brownian dynamics</td>
<td>Kinetic Monte Carlo</td>
</tr>
<tr>
<td></td>
<td>Molecular dynamics</td>
<td></td>
</tr>
<tr>
<td>Particle</td>
<td></td>
<td>Electronic structures</td>
</tr>
<tr>
<td>simulation</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 2. Comparison of the frequently used terminologies.

<table>
<thead>
<tr>
<th>Terminology</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lifting operator</td>
<td>[95]</td>
</tr>
<tr>
<td>Prolongation operator</td>
<td>[26]</td>
</tr>
<tr>
<td>Reinitialization</td>
<td>[106, 5]</td>
</tr>
<tr>
<td>Reconstruction operator</td>
<td>[55]</td>
</tr>
<tr>
<td>Compression operator</td>
<td>[55]</td>
</tr>
<tr>
<td>&quot;Equation-free&quot;</td>
<td>[95]</td>
</tr>
<tr>
<td>Solving equations without equations</td>
<td>[29]</td>
</tr>
<tr>
<td>&quot;On-the-fly&quot; calculation</td>
<td>[6]</td>
</tr>
<tr>
<td>Concurrent computing</td>
<td>[6]</td>
</tr>
<tr>
<td>Parameter passing</td>
<td></td>
</tr>
<tr>
<td>Microscopically-informed modelling</td>
<td></td>
</tr>
<tr>
<td>Pre-computing</td>
<td>[6]</td>
</tr>
<tr>
<td>Serial computing</td>
<td>[6]</td>
</tr>
<tr>
<td>Other terminologies</td>
<td>Termination adopted here</td>
</tr>
</tbody>
</table>
First principle-based molecular dynamics (FPMD)

Macroscale: Molecular Dynamics of atoms (nuclei)

Microscale: Quantum mechanics of electrons
MD: \( M_I \ddot{R}_I = -\nabla_{R_I} V_0(R_1, \ldots, R_N) \)

Question: \( V_0 = ? \)

\[ V_0 = \langle \psi_0 | \hat{H}_{ee} | \psi_0 \rangle + \sum_{I,J} \frac{Z_i Z_j}{|R_I - R_J|} \]

\( \psi_0 = \psi_0(r_1, r_2, \ldots, r_M) = \text{ground state of electrons} \)

\[ \hat{H}_{ee} = \sum -\frac{1}{2} \nabla^2_{r_i} + \sum \frac{1}{|r_i - r_j|} + \sum v(r_i) \]

\[ v(r_i) = -\sum \frac{Z_I}{|r_i - R_I|} \]

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
ad hoc

\[ \text{stored-energy density} = M \]

\[ \sum_{n} \min \int \rho x p (n \Delta) M \]

Traditional approach: \( n \) displacement field

Goal: Compute macroscopic deformation of solid

\[ \text{position of } j\text{-th atom} = \dot{x}_j \]

\[ (\dot{x}_j, \dot{x}_j, \dot{x}_j) \Lambda + (\dot{x}_j, \dot{x}_j, \dot{x}_j) \Lambda \dot{x}_{\Sigma} = \mathbf{E} \]

Given: Molecular mechanics model

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

Quasi-continuum Method
Limited to statics, zero temperature

3. Adaptive mesh refinement

Mixed: "Ghost force"

Nonlocal: summation over clusters

\[ \forall n \Delta = \forall \\{n \in \mathbb{N}\} \text{, } \sum \approx \mathcal{E} \]

Local: use Cauchy-Born rule

2. Summation rule

\[ \forall n \sum_0^\alpha (x) \approx \mathcal{E} \]

1. Selecting representative atoms

\[ \cdots + \sum_0^\alpha (x, x) + (x, x, x) \sum \approx \mathcal{E} \]

Microscopic model: \( \mathcal{E} \) (Tadmor et al. 1996)

Quasicontinuum Method
varies according to the severity of the variation in the deformation gradient. The density of the repoms, which are then meshed by linear triangular elements in (q), is shown in (q).

Figure 2: Selection of repoms from all the atoms near a dislocation core are shown in (q).
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, \( \sigma = \sigma(A_t) = \sigma(D) \)

\( u = \) displacement,
\( A = \nabla u = \) deformation gradient
\( v = u_t = \) velocity
\( D = \frac{1}{2}(\nabla v + \nabla v^T) = \) rate of strain
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 \( x_i^0 x_j^0 \) in \( \Omega_0 \)

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

\( = \) Piola-Kirchhoff stress

\( T > 0 : \quad \text{"entropic contribution"} \)
The I-K formula (MD) needs to be localized:

Irving-Kirkwood (1950)

\[ \left\langle \chi_P(x - i^b(b - \gamma) + i^b\gamma) \int \left( \frac{\hat{\beta} \otimes (\hat{b} - i^b)}{\hat{I}} \right)^{\frac{2}{\xi}} \right\rangle + \left\langle (x - i^b)\gamma'(d \otimes d) \frac{i^w}{\hat{I}} \right\rangle = (1 \cdot x)\Sigma \]

\[ 0 = 2 \cdot \Delta + i^w \]

\[ \left\langle (x - (1)^i^b)\gamma(1)^d \frac{i^w}{\hat{I}} \right\rangle = (1 \cdot x)\Sigma \]

Conservation of momentum (MD):

Connection of macro and micro models
Renitialization

Periodic BC on the dynamically changing box

$\nu_{\nu} = \frac{1p}{\nu_{\nu}}$

Deforming the simulation box

\[\begin{pmatrix} 0 & 0 & 0 \\ 0 & \nu - c & 0 \\ 0 & q & 0 \end{pmatrix} = \nu = n\Delta\]

Constant rate of strain \(\nu\)
\[ \mathcal{P}(i) \int_0^L \frac{L - \mathcal{I}}{\mathcal{I}} = \tau_2 \]

\[ \mathcal{U} \ni \{ b'' b \} \text{ if only one } \mathcal{U} \ni \{ b'' b \} \text{ if } 0 \]

\[ \mathcal{U} \ni \{ b'' b \} \text{ if } 1 \]

\[ \mathcal{U} : \text{Area of the simulation box} \]

\[ \mathcal{H} \otimes (f b - i b) \frac{\mathcal{U} \mathcal{Z}}{\mathcal{I}} + (d \otimes d) \frac{\mathcal{U} \mathcal{W}(i) \mathcal{U} \mathcal{Z}}{\mathcal{I}} = (i) \tau_2 \]

Average the momentum flux over space and time:

\[ \mathcal{N}(x - f b (y - 1) + i b y) \int_0^L \frac{\mathcal{U} \mathcal{Z}}{\mathcal{I}} + (x - i b) \frac{\mathcal{U} \mathcal{W}(i) \mathcal{U} \mathcal{Z}}{\mathcal{I}} = (i x) \tau_2 \]

Extracting the stresses using \( K \) formula
STLDD algorithm (Hoover, Ladd)

Lees-Edwards BC (1972)

\[ 0 = (\lambda', x) w, \quad 0 = (\lambda', x) v, \quad \Lambda q = (\lambda', x) n \]

constant rate of strain MD in 1D (pure shear)
Example of stress: Simple LJ Fluids

\[ \dot{\gamma} = 0.810^3, \ \lambda = 1.46, k^8 \]

\[ \rho = 1.1^3 \]

\[ \gamma = \frac{N}{A} \]

\[ \mu = \text{shear rate} \]

\[ \eta = \text{viscosity} \]

\[ \mu \dot{\gamma} = p \]

Example of stresses: Simple LJ Fluids
0 = m = \lambda, \dot{\lambda} = n

Study of the Constitutive Relation for Polymeric Fluids
Other example of shear-thinning fluids: Ketchup, paint, blood

\[ (N)^{u/2} \]

Maximum relaxation time

\[ \zeta = u \left( (N)^{u/2} + 1 \right)^0 \]

\[ \zeta = u \]

Zero-shear viscosity

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

For small \( (N)^0 u \sim u \)

For large \( (N) \infty u \sim u \)

\( N < 5 \) Shear-thinning

\( N > 5 \) Newtonian

Shear viscosity vs. shear rate
No-slip boundary condition is invalid near the contact line.

Example of multiscale method: Contact line dynamics
Example of Slip Models:

\[
\begin{cases}
1^+ & \text{between Fluid A and B} \\
1^- & \text{otherwise}
\end{cases} = \mathcal{S}
\]

\[
\left( \frac{\partial}{\partial \nu} \mathcal{S} - \frac{\partial}{\partial \nu} \mathcal{S} \right) \mathcal{A}_g = (\rho)_{\text{IIA}}
\]
Tangential stress near the CL & Contact angle are calculated from MD

Surface tension is smoothed out to the neighboring points (Peshkin)

Spatial discretization on staggered grid; The interface is represented

\[ Ix^0f - \frac{1}{\gamma} (u \otimes u - I) \lambda + (nA + nA) n' - Id + n \otimes n \sigma = 1 \]

\[
\begin{align*}
\begin{aligned}
n &= \chi \\
0 &= n \cdot \Delta \\
0 &= \Delta + n \cdot n \sigma 
\end{aligned}
\end{align*}
\]

Multiscale modeling of contact line dynamics
Multiscale modeling of contact line dynamics

- Imposed alternatively
- The constraints in horizontal and vertical strips are

the boundary in x direction
- Particle species needs to be changed when crossing

Periodic in Y

Sampling Region

Confined MD

Repulsive force
Validation of the multiscale method
system size: 1500 × 500
λ = 3.7
η = 2.0
ρ = 0.81

Dynamics of contact angle

Dynamics of interface

External force

(1) \( f = \sigma \)

Application to a larger system: Asymmetric fluid-solid interaction
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