Simulations of real complex systems: computational science comes of age

PICS Inaugural Symposium
UPenn - October 10, 2013
Multiscale models for complex physical systems

The Nobel Prize in Chemistry 2013
Martin Karplus, Michael Levitt and Arieh Warshel

"for the development of multiscale models for complex chemical systems"
October 9, 2013

PICS – October 10, 2013
Microscale

Macroscale

Mesoscale

Length scale (from nm to mm)

Time scale (from as to ms)

EXPERIMENT

MATHEMATICAL

MODELING

EXPERIMENT
Multiple length/time scales: brittle fracture (corrosion)

- Quantum mechanics (ions + electrons)
- Classical dynamics (atoms)
- Classical Dynamics (defects)
- Effective interatomic forces (springs)
- Effective defect interactions
- Interactions from first principles
- Constitutive laws
Density Functional Theory

Many-body:

\[
\left( \hat{H} - E \right) \psi (r_1 \sigma_1, r_2, \sigma_2, \ldots) = 0
\]

: Unsolvable

Hohenberg & Kohn (PRB, 1964):

\[
E [V(r)] = \min_{\rho(r)} E' [V(r); \rho(r)]
\]

Kohn & Sham (PRB, 1965):

\[
E' [V(r); \rho(r)] = T_s[\rho] + E_{\text{Hart}}[\rho] + \int \rho(r) V(r) dr + E_{\text{xc}}[\rho]
\]

\[
\left( \hat{H}_{\text{KS}} - \epsilon_i \right) \psi_i(r) = 0
\]

Kohn, Pople
Nobel Prize in Chemistry, 1998
Brittle fracture of silicon
Abraham, Broughton, Bernstein, Kaxiras, PRB (1998)

CLASSICAL ATOMISTICS

CONTINUUM MECHANICS
Ions + electrons: chemical bonds

QUANTUM MECHANICS
The need for alternative energy sources

Global carbon dioxide emissions from human activities, 1750-2004

Global Temperatures

Positive proof of global warming.

1990 zones are by the United States Department of Agriculture. 2006 zones are by the National Arbor Day Foundation.

The challenge of sustainable energy

Time and resources running out

Report of Intergovernmental Panel on Climate Change
2007 Nobel Peace Prize (shared with A. Gore)
Light absorption by hybrid cells

The Problem: materials for carrier transport with large band gaps

TiO$_2$ gap = 3.2 eV (200 nm < $\lambda$ < 400 nm)

solar spectrum
The dye-sensitized (3rd generation) solar cell

The Principle: Separate light-absorption and charge collection processes
The dye-sensitized solar cell (DSSC)

Major issues:
- stability
- efficiency

Incident Photon to Current Efficiency

\[ \text{IPCE}(\lambda) = \text{LHE}(\lambda) \times \Phi(\text{inj}) \times \eta(\text{c}) \]

LHE = Light Harvesting Efficiency
\( \Phi(\text{inj}) = \) electron injection efficiency
\( \eta(\text{c}) = \) charge collection efficiency
Main issue: coupled electron-ion dynamics

Previous work:
-Schroedinger eq. with model Hamiltonian
  Thoss, Miller, Stock, JCP (2000);
  Rego & Batista, JACS (2003);
-semiempirical Hamiltonian (tight-binding)
  Allen et al., JMO (2003);
-ground state DFT + TDDFT
  Prezhdo et al., PRL (2005); JACS (2007);

self-consistent TDDFT with atomic motion

Coupled electron-ion dynamics

\[
\begin{align*}
    i\hbar \frac{\partial \phi_j(r, t)}{\partial t} &= -\frac{\hbar^2}{2m} \nabla^2_r \phi_j(r, t) + v_{\text{ext}}(r, t) + \int \frac{\rho(r', t)}{|r - r'|} \, dr' - \sum_I \frac{Z_I}{|r - R_I^d|} + v_{xc}[\rho](r, t) \\
    M_J \frac{d^2 R_{jI}^d(t)}{dt^2} &= -\nabla_{R_{jI}^d} \left[ V_{\text{ext}}^J(R_{jI}^d, t) - \int \frac{Z_J \rho(r, t)}{|R_{jI}^d - r|} \, dr + \sum_{I \neq J} \frac{Z_J Z_I}{|R_{jI}^d - R_{jI}^d|} \right]
\end{align*}
\]

Propagation of electrons in time (TDSE) + Ehrenfest dynamics for ions

Transport: $10^{-12} \text{ s}$
Electron and hole motion in DSSC
"Designer" dyes: Predict properties of new dyes (not yet tried in experiments)
D-π-A Dye System Containing Cyano-Benzonic Acid as Anchoring Group for Dye-Sensitized Solar Cells
Masataka Katono, Takeru Bessho, Sheng Meng, Robin Humphry-Baker, Guido Rothenberger, Shaik M. Zakeeruddin, Efthimios Kaxiras, and Michael Gratzel
Langmuir 2011, 27, 14248–14252
Artificial Nano Tree (based on QM simulations)

Cheng et al., JPCC (2008).
Acute Myocardial Infarction (heart attack)

Deaths in USA: out of ~2.5 M per year total,
- 35% blood flow obstruction (80% heart, 20% brain)
  UNPREDICTABLE
- 25% cancer (all types)
Formation and evolution of plaques

ESS = Endothelial Shear Stress, ACCESSIBLE ONLY BY SIMULATION
Vasculoprotective Vascular adhesion of lipoproteins & inflammatory cells
Inflammatory response & Feedback

Cholesterol (HDL, LDL)  White blood cells
Challenge: Multi-scale hemodynamics
Fluid dynamics by cellular automata: Lattice Boltzmann Equation (LBE)

Bhatnagar-Gross-Krook algorithm

Reproduces the physics of fluid dynamics (Navier-Stokes equation)
Fluid properties:

Fluid density

Momentum (flow)

Stress Tensor

Wall Stress
Red Blood Cell in Motion

- Tumbling (Flipping Coin)
- Tank Treading
- Deformation
- Lift $\alpha \gamma$

WALL
Definition of “particles” (cells, proteins, …)

\[ \tilde{\delta}_{\vec{x}}(x - R) = \prod_{\alpha=x,y,z} \tilde{\delta}_{\xi}(x_{\alpha} - R_{\alpha}) \]

\[ \varphi(x, R) = -\gamma(V - u(x))\tilde{\delta}_{\xi}(x - R) \]

\[ F^H = \sum_x \varphi = -\gamma(V - \tilde{u}) \]

\[ \tilde{u} = u \ast \tilde{\delta}_{\xi} \]

\[ \Delta f_p = -\frac{w_p}{c^2 c_p} \cdot \sum_R \varphi \]
Equations of motion:

\[
\frac{d\Psi}{dt} = \left( M \frac{dV}{dt} \right) = \left( F + F^H \right) = \Phi + \Phi^H
\]

\[
\Phi^H_{6\times1} = \Gamma_{6\times6} \Psi^*_{6\times1} + \Delta_{6\times3\times3} : E_{3\times3}
\]

\[
\Psi^* = \begin{pmatrix} V - u \\ \Omega - \omega \end{pmatrix}
\]

Brenner et al. (1972) Brady & Bossis (1989)

\[\Gamma\text{ and } \Delta\text{ depend on the whole configuration}
\]

Pair-wise superposition

\[O(N^3)\text{ complexity!}\]

\[
\Gamma = \text{Grand Resistance matrix}
\]

\[
\Delta = \text{Shear Resistance matrix}
\]

\[
E = \text{Strain tensor}
\]

\[
u = \text{Fluid velocity @center}
\]

\[
\omega = \frac{1}{2} \partial \times u = \text{Fluid vorticity @center}
\]
Fluid-particle coupling:

\[
(\partial_t + v \cdot \partial_x) f = -\omega (f - f^{eq}) - \frac{1}{M} \sum_R F^H \cdot \partial_v f
\]

\[
\frac{d}{dt} V = \frac{1}{M} (F + F^H)
\]

\[
F^H = -\gamma [V - u(x,\{R,V\})] \delta(x - R)
\]

Momentum exchange (Newton’s 3rd law)
ESS Calculation in patient-specific arterial tree
Full arterial tree (10⁹ grid points) with RBC’s (10⁸ cells)
Hemodynamics Pipeline

Patient Data → Data Segmentation → Data Preparation

Parallel Code: MUPHY & HARVEY

Output visualization
Multiscale Hemodynamics Team

Course Information

Physical Sciences 12b: Electromagnetism and Statistical Physics from an Analytic, Numerical and Experimental Perspective
Harvard College/GSAS: 82209
Fall 2013–2014
Efthimios Kaxiras
Location: Science Center B
Meeting Time: Tu., Th., 11:30–1
Exam Group: 13,14

This is the second term of a two-semester introductory sequence that uses a combination of analytic and numerical methods to understand physical systems, to analyze experimental data, and to compare data to models. Topics include electrostatics and magnetostatics, electromagnetic fields, optics [all topics illustrated with applications to current technological and societal challenges], and an introduction to the physics of many-body systems and their aggregate properties such as entropy, temperature and pressure. The course is aimed at second year students who have an interest in pursuing a concentration in the sciences and/or engineering. The course structure includes lecture, discussion and laboratory components.

Note: May not be taken for credit by students who have passed Physics 15b or Physics 15c. This course, when taken for a letter grade, meets the General Education requirement for Science of the Physical Universe or the Core area requirement for Science A.

Prerequisite: Physical Sciences 12a
The SEAS graduate program in Computational Science and Engineering (2013-14 inaugural Academic Year)

Advisory Board: experts from Industry and National Labs (IBM, Nvidia, Intel, Microsoft, Goldman Sachs, ... Lawrence Livermore, Los Alamos, ...)

Master’s programs built around set of learning outcomes

Core and Elective courses
what is a Master’s degree in CSE?

• Master of Science (S.M.): total of 8 courses including CSE core courses
• Master of Engineering: total of 16 courses including two semesters of research (Thesis)

• Secondary Field and S.M. are appropriate for Ph.D. students wanting to apply computational methods to a problem in a domain of science, engineering or social science
core courses

AM205 Advanced Scientific Computing: Numerical Methods

offered in fall
core courses

**CS205** Computing Foundations for Computational Science

offered in fall
core courses

AM207 Advanced Scientific Computing:
Stochastic Optimization Methods

offered in spring
core courses

CS207 Systems Design for Computational Science

offered in spring
electives

AM272r Kinetic Methods for Fluid: Theory and Applications

AM274 Computational Design of Materials

AM275 Computational Fluid Dynamics
Learning outcomes

1. state-of-the-art modeling and simulation approaches
2. techniques for evaluating and comparing multiple computational approaches
3. skills in collaboration, code implementation and development of robust, reliable software
4. new methods for modeling big data and complex systems
5. how to take advantage of parallel and distributed computing
6. advanced data analysis and visualization methods
7. parallel programming and “parallel thinking”
Congratulations David!
Warm welcome to PICS!
Best wishes for success and growth (we’re counting on it)!

42