Introduction

Lecture 1

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Subject structure and grading scheme

**Part I:** Continuum and particle methods (Markus Buehler)
*Lectures 2-13*

**Part II:** Quantum mechanics (Jeff Grossman)
*Lectures 14-26*

*The two parts are based on one another and will be taught in an integrated way*

The final grade will be based on:
**Homework (50%) and exams (50%)**
A few things we’d like you to remember…

- The goal is to provide you with an excellent foundation for modeling and simulation, beyond the applications discussed in IM/S.

- Our goal: Discover the world of Modeling and Simulation with you – using a bottom-up approach.

We will cover multiple scales -- the atomic scale, using Newton’s laws, statistical mechanics and quantum mechanics (involving electrons), as well as continuum methods.

You will be able to apply the knowledge gained in IM/S to many other complex engineering and science problems
Subject content: Big picture

- Subject provides an introduction to modeling and simulation.

- Scientists and engineers have long used models to better understand the system they study, for analysis and quantification, performance prediction and design. However, in recent years – due to the advance of computational power, new theories (Density Functional Theory, reactive force fields e.g. ReaxFF), and new experimental methods (atomic force microscope, optical tweezers, etc.) – major advances have been possible that provide a fundamentally new approach to modeling materials and structures.

- This subject will provide you with the relevant theoretical and numerical tools that are necessary to build models of complex physical phenomena and to simulate their behavior using computers.

- The physical system can be a collection of electrons and nuclei/core shells, atoms, molecules, structural elements, grains, or a continuum medium: As such, the methods discussed here are VERY FLEXIBLE!

- The lectures will provide an exposure to several areas of application, based on the scientific exploitation of the power of computation,
Engineering science paradigm: Multi-scale view of materials

Macroscale structural engineering

Ultrascale structural engineering


Characteristic scale of technology frontier (materials)

Axes
Weapons
Equipment
tools
weapons
Machines
Mass production
Building
materials
Transistors
Integrated circuits
Agriculture
Industrialization
IT revolution
Bio-X revolution
AFM, SEM
CNTs as electronic
devices
Biology &
nanotech

Fig. 1.1 in Buehler, Markus J. Atomistic Modeling of Materials Failure. Springer, 2008. © Springer. All rights reserved. This content is excluded from our Creative Commons license. For more information, see http://ocw.mit.edu/fairuse.
Content overview

I. Particle and continuum methods
   1. Atoms, molecules, chemistry
   2. Continuum modeling approaches and solution approaches
   3. Statistical mechanics
   4. Molecular dynamics, Monte Carlo
   5. Visualization and data analysis
   6. Mechanical properties – application: how things fail (and how to prevent it)
   7. Multi-scale modeling paradigm
   8. Biological systems (simulation in biophysics) – how proteins work and how to model them

II. Quantum mechanical methods
   1. It’s A Quantum World: The Theory of Quantum Mechanics
   2. Quantum Mechanics: Practice Makes Perfect
   3. The Many-Body Problem: From Many-Body to Single-Particle
   4. Quantum modeling of materials
   5. From Atoms to Solids
   6. Basic properties of materials
   7. Advanced properties of materials
   8. What else can we do?

Lectures 1-13
Lectures 14-26
Engineering science paradigm: Multi-scale view of materials

“molecular” (explicitly resolve molecules/atoms)
Molecular Dynamics

“continuum” (matter infinitely divisible, no internal structure)
e.g. finite element methods

“quantum” (explicitly resolve electrons);
e.g. Density Functional Theory
A few important concepts in modeling and simulation

*What is the difference between modeling and simulation?*
Modeling and simulation

- The term *modeling* refers to the development of a mathematical representation of a physical situation.

- On the other hand, *simulation* refers to the procedure of solving the equations that resulted from model development.
What is a model?

Mike Ashby (Cambridge University):

- A model is an idealization. Its relationship to the real problem is like that of the map of the London tube trains to the real tube systems: a gross simplification, but one that captures certain essentials.
What is a model?

Mike Ashby (Cambridge University):

- The map *misrepresents distances and directions*, but it elegantly displays the connectivity.

- The *quality or usefulness in a model* is measured by its ability to capture the governing physical features of the problem. All successful models unashamedly distort the inessentials in order to capture the features that really matter.

- At worst, a model is a concise description of a body of data. At best, it captures the essential physics of the problem, it illuminates the principles that underline the key observations, and it predicts behavior under conditions which have not yet been studied.
What is a simulation?

- *Simulation* refers to the procedure of solving the equations that resulted from model development.

- For example, numerically solve a set of differential equations with different initial/boundary conditions.

\[
\frac{\partial u}{\partial t} - \alpha \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) = 0
\]

+ BCs, ICs
Introduction part I

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## Content overview

### I. Particle and continuum methods

1. Atoms, molecules, chemistry
2. Continuum modeling approaches and solution approaches
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4. Molecular dynamics, Monte Carlo
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6. Mechanical properties – application: how things fail (and how to prevent it)
7. Multi-scale modeling paradigm
8. Biological systems (simulation in biophysics) – how proteins work and how to model them

### II. Quantum mechanical methods

1. It’s A Quantum World: The Theory of Quantum Mechanics
2. Quantum Mechanics: Practice Makes Perfect
3. The Many-Body Problem: From Many-Body to Single-Particle
4. Quantum modeling of materials
5. From Atoms to Solids
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Lectures 2-13

Lectures 14-26
Multi-scale view of materials

Macroscale structural engineering

Ultrascale structural engineering


Example application: Stiffness of materials (Young’s modulus)

**Objective:** Illustrate the significance of multiple scales for material behavior and introduce multi-scale modeling paradigm
Beam deformation problem – continuum model

Governing equation (PDE)

$$-EI_{zz} \frac{\partial^4 u_z}{\partial x^4} + q_z = 0$$

Geometry

$$I_{zz} = \frac{bh^3}{12}$$

BC - load:

$$\rho g A$$

Integration & BCs

$$u_z(x) = -\frac{\rho g A}{24EI_{zz}} x^4$$

Question: Displacement field

$E$ is parameter called “Young’s modulus” that relates how force and deformation are related (captures properties of material)
How to determine Young’s modulus $E$?

Measurement (laboratory):

Rod/beam (e.g. plastic, metal, nanowire)

$F = k_s \Delta u$

$E = \frac{Lk_s}{A}$

Young’s modulus $E$ (~stiffness=proportionality between force and displacement)
How to determine $E$? - alternative approach

Atomistic simulation – *new engineering paradigm*

*Idea:* Consider the behavior of a collection of atoms inside the beam as deformation proceeds

Image from Wikimedia Commons, [http://commons.wikimedia.org](http://commons.wikimedia.org).
Molecular dynamics simulation

- Newton’s laws: $F = ma$
- Chemistry: Atomic interactions – calculate interatomic forces from atomic interactions, that is, calculate $F$ from energy landscape of atomic configuration (note that force and energy are related…)

![Diagram of molecular dynamics simulation](image)
Linking atomistic and continuum perspective

- Atomistic viewpoint enables us to calculate how force and deformation is related, that is, we can predict $E$ once we know the atomic structure and the type of chemical bonds.

- Example, in metals we have metallic bonding and crystal structures – thus straightforward calculation of $E$.

- Atomistic models provide fundamental perspective, and thereby a means to determine (solely from the atomistic / chemical structure of the material) important parameters to be used in continuum models.

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Quantum mechanics

- Deals with **fundamental view** of chemical bonding, based on electrons in atoms

\[ \text{diene} + \text{dienophile} \]

conjugated (substituted) diene + (substituted) olefin \( \rightarrow \) (substituted) cyclohexene

“Schroedinger equation”

\[
\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m}{\hbar^2} (E - V)\psi = 0
\]
Developing a potential energy from quantum mechanics

\[ \frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m}{\hbar^2} (E - V) \psi = 0 \]

JAVA Applet

Example: Stretching nanowire

\[ F = k_s \Delta u \]

\[ E = \frac{Lk_s}{A} \]

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Multi-scale simulation paradigm

Molecular model (fundamental) → Parameters (Young’s modulus) → Use in model with PDE that involves Young’s modulus as parameter

“continuum scale”
Matter is indefinitely Divisible

div σ + f = 0

Image by MIT OpenCourseWare.

Courtesy of Elsevier, Inc. Used with permission.
Beam deformation problem – continuum model

**Question:** Displacement field

**Governing equation (PDE)**

\[-EI_{zz} \frac{\partial^4 u_z}{\partial x^4} + q_z = 0\]

**Geometry**

\[I_{zz} = \frac{bh^3}{12}\]

**BC - load:**

\[\rho g A\]

\[u_z(x) = -\frac{\rho g A}{2EI_{zz}} x^4\]

*E* = parameter (obtained from atomistic simulation)

*E* is parameter called “Young’s modulus” that relates how force and deformation are related (captures properties of material)
Applications of continuum methods
Cloth modeling for animated movies


Aivazis, Lombeyda and RR, 2003
Airbag deployment dynamics

Image courtesy of High Contrast. License: CC-BY.

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Benefits of atomistic models
Other material properties

- Atomistic models are not limited to calculation of $E$ (or generally, elastic properties)
- Atomistic models also enable us to predict failure, fracture, adhesion, diffusion constants, wave speeds, phase diagram (melting), protein folding (structure), …

Glass – brittle (breaks easily)  Metal – ductile (deformable)
Failure of materials and structures

**Failure** = uncontrolled response of a structure, often leading to malfunction of entire device, system

- **Earthquake**
- **Collapse of buildings**
- **Engineering materials fracture** (ceramics, tiles)
- **Bone fracture**

Cost of failure of materials: >>$100 billion (1982)
Failure of materials observed at macroscale is due to repeated breaking, shearing, tearing of bonds at atomistic scale.

Nanoscopic response of material’s building block is key for materials failure.
http://web.mit.edu/mbuehler/www/research/supersonic_fracture.mpeg
Supersonic fracture: Discovered in atomistic simulation on supercomputers

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Please see Fig. 2 in Petersan, Paul J., Robert D. Deegan, M. Marder, and Harry L. Swinney. "Cracks in Rubber under Tension Exceed the Shear Wave Speed." Phys Rev Lett 93 (2004): 015504.
Failure of biological structures in diseases

Failure of materials is critical for understanding function and malfunction of biology

**Example:** Rapid aging disease *progeria* - Single point mutations (changes) in protein structure causes severe diseases

Cell nucleus loses mechanical stability under loading (heart, muscles)

Patient

Fracture in cell's nucleus
Created under mechanical deformation

Failure of protein molecules
Building blocks of life

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How structural building blocks of cells break

- Genetic diseases
- Molecular mechanisms of biology

Courtesy of National Academy of Sciences, U.S.A. Used with permission.
Unfolding of titin molecule

Titin I27 domain: Very resistant to unfolding due to parallel H-bonded strands

Keten and Buehler, 2007
Folding of beta-sheet protein structure
S. Keten and M.J. Buehler, *in submission*
A New Approach to Molecular Simulation

Vijay Pande, Associate Professor of Chemistry, Structural Biology, and Computer Science, Stanford University

Folding@home distributed computing
http://folding.stanford.edu/
Integration with experimental techniques

For most applications, we will use a website-driven simulation framework developed in collaboration with MIT’s Office for Undergraduate Education

nanoHUB: https://nanohub.org

More than 160 tools: https://nanohub.org/resources/tools

Technical assistance: Justin Riley
Example: Stretching nanowire

\[ F = k_s \Delta u \]

\[ E = \frac{Lk_s}{A} \]