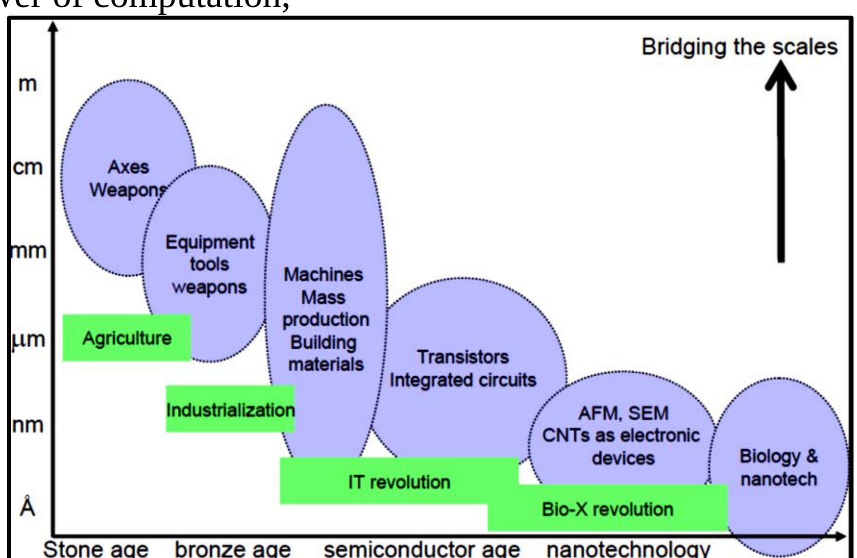
Lectures (6-7): Modeling and Simulation (Examples and Application

6.1 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!*
- This lecture will provide an exposure to several areas of application, based on the scientific exploitation of the power of computation,

6.1.1 Characteristic scale of technology frontier (materials)



6.1.2 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

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.

6.1.3 What is a simulation?

- S*imulation* 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.

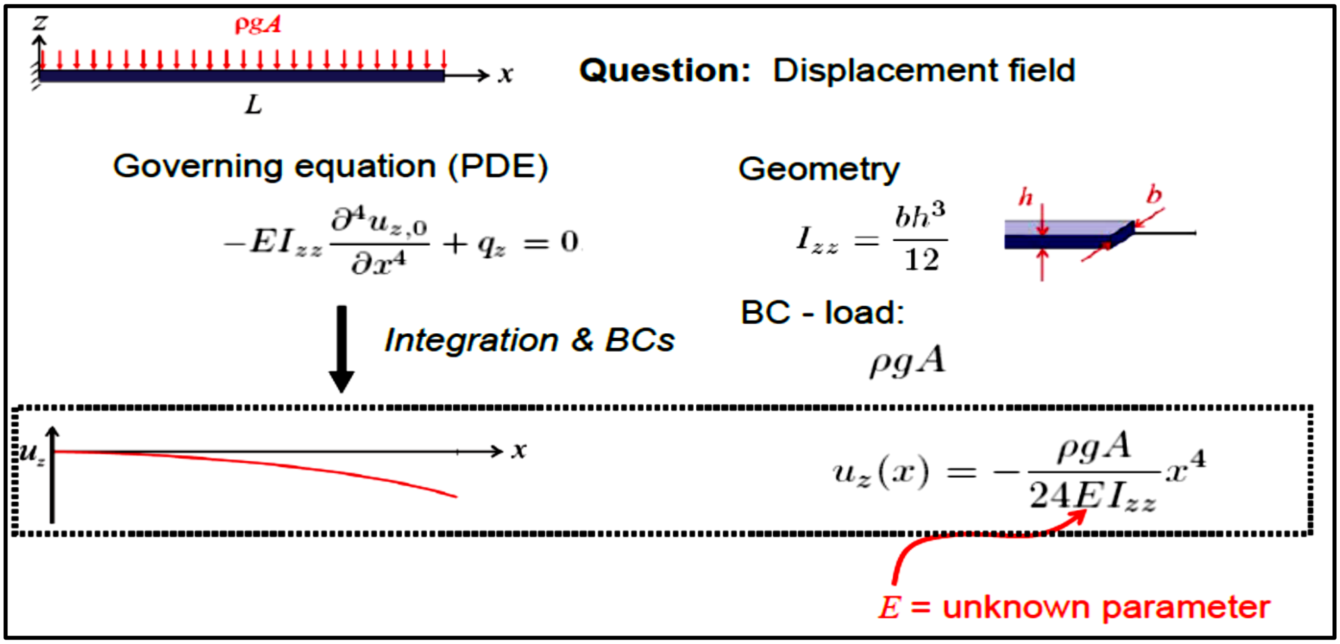
$$\frac{\partial u}{\partial t} - \alpha\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right) = 0$$

$$+ \text{ BCs, ICs}$$

6.2 Beam deformation problem –continuum model

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

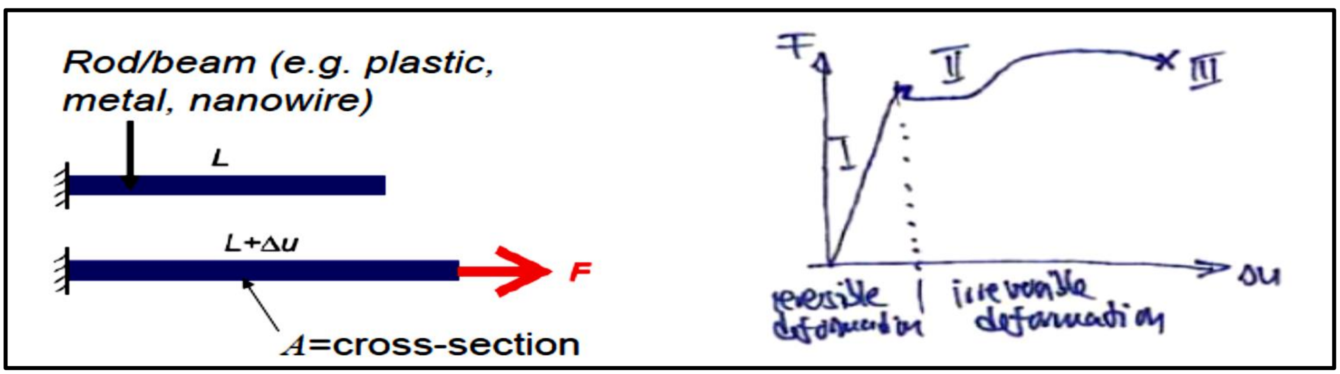
Objective: Illustrate the significance of multiple scales for material behavior and introduce multi-scale modeling paradigm



E is parameter called "**Young's modulus**" that relates how force and deformation are related (captures properties of material)

6.2.1 How to determine Young's modulus *E*?

Measurement (laboratory):



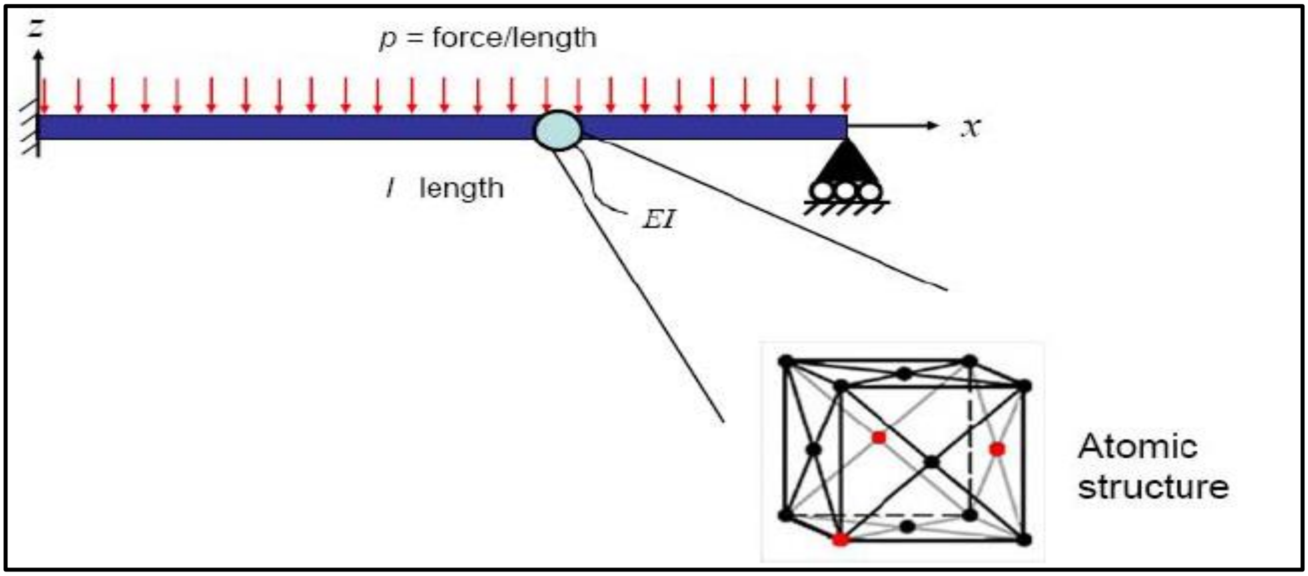
$$F = k_s \Delta u$$

$$E = \frac{L k_s}{A}$$

Young's modulus *E* *(~stiffness=proportionality between force and displacement)*

6.2.2 How to determine E? -alternative approach

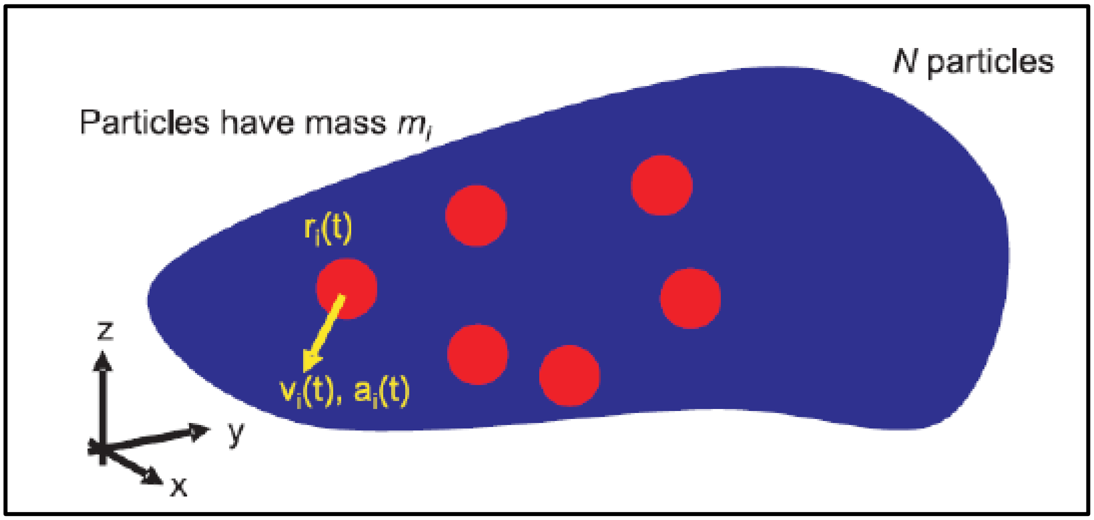
Atomistic simulation *–new engineering paradigm*



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

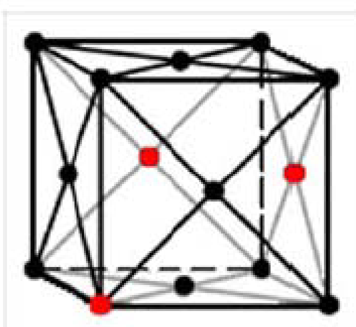
6.2.3 Molecular dynamics simulation

- **Newton's laws:** *F*=m*a*
- **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…)



6.2.4 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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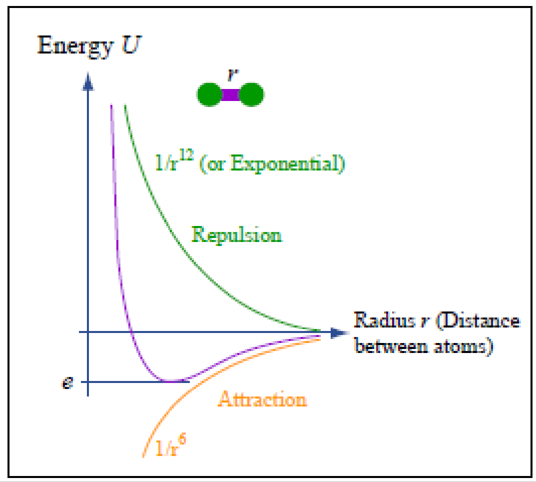
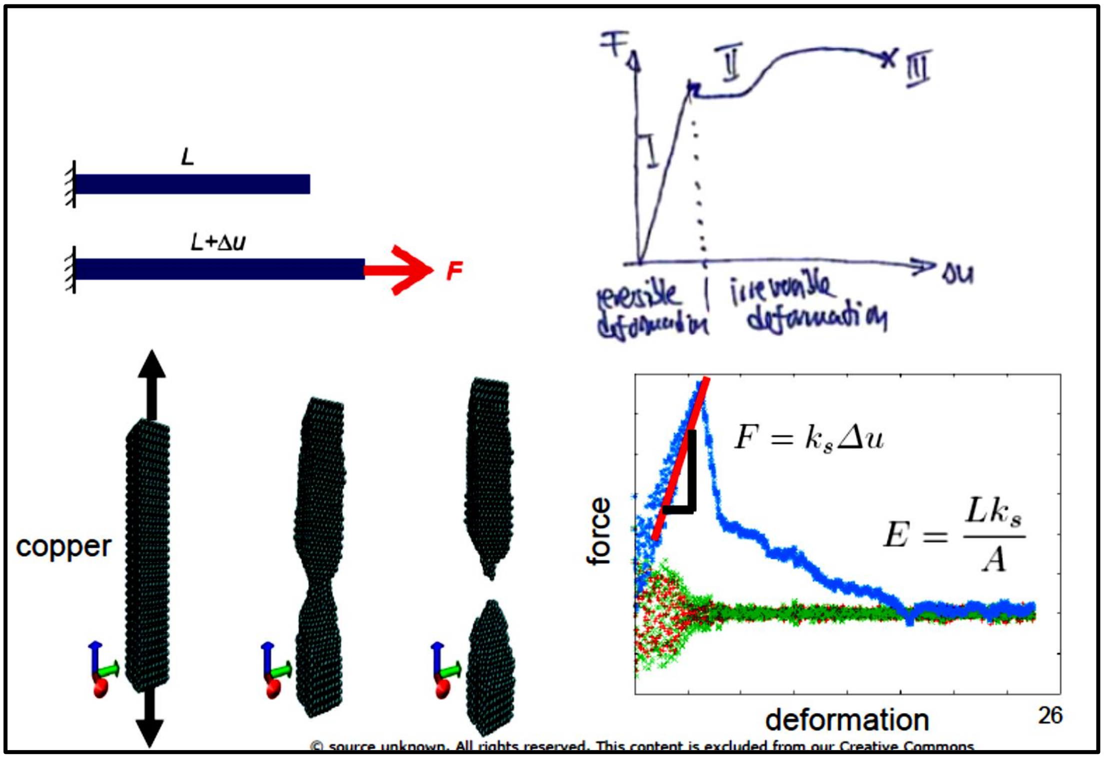
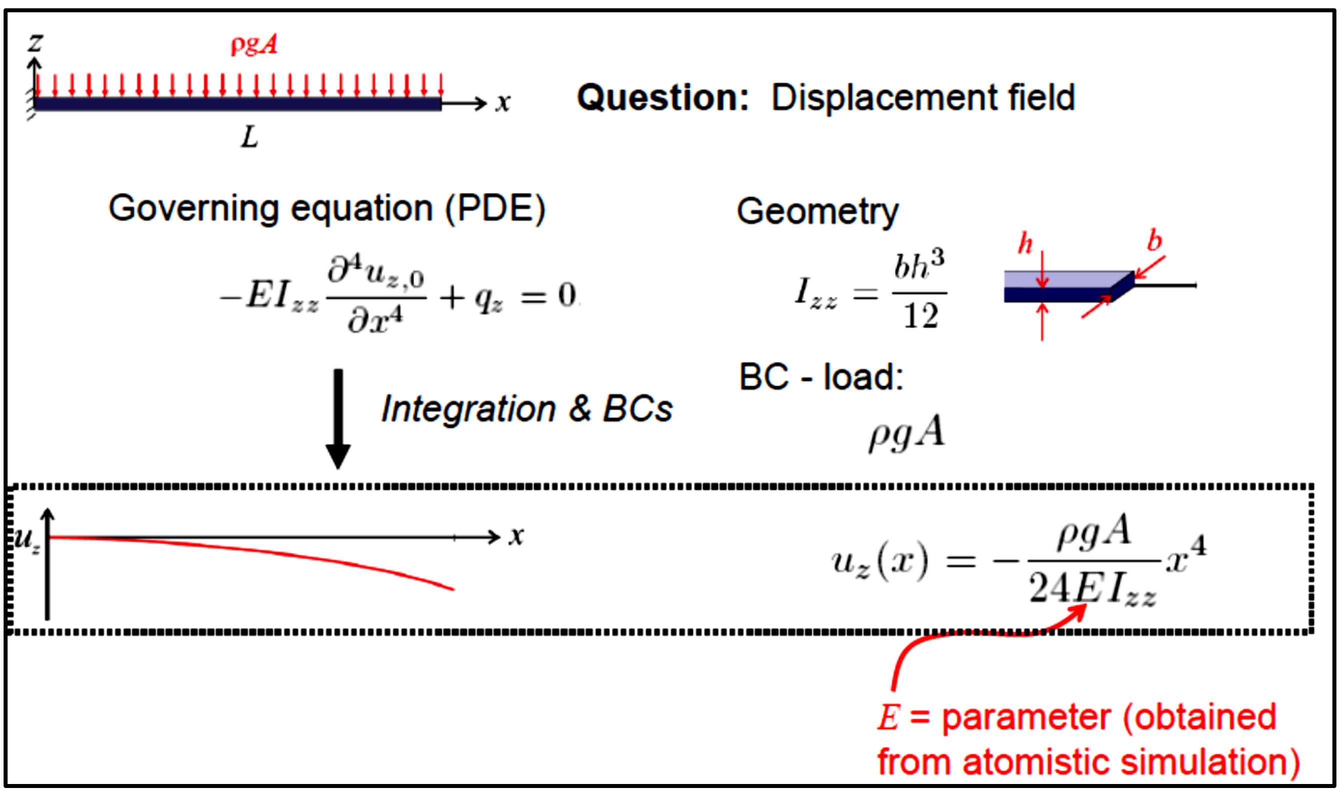


6.2.5 Example: Stretching nanowire



6.2.6 Beam deformation problem –continuum model



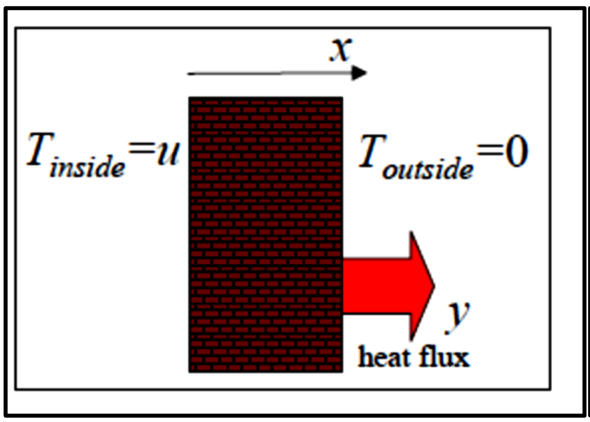
BCs *AE* is parameter called “Young’s modulus” that relates how force and deformation are related (captures properties of material)

- 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), …

6.3 Linear PDE System

Example: PDE models

- Include functions of spatial variables
  – electromagnetic fields
  – mass and heat transfer
  – fluid dynamics
  – structural deformations
- Example: sideways heat equation

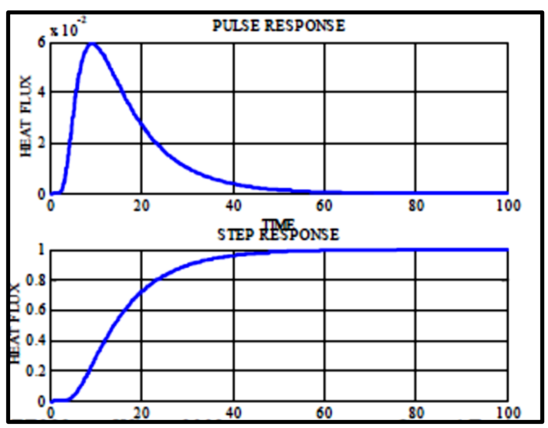


$$\frac{\partial T}{\partial t} = k\frac{\partial^2 T}{\partial x^2}$$

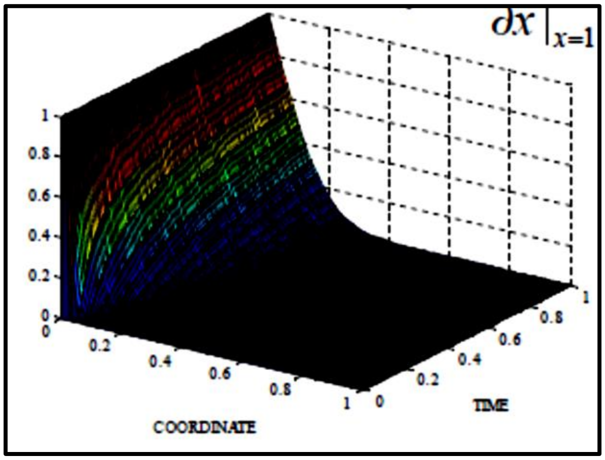
$$T(0) = u; \qquad T(1) = 0$$

$$y = \left.\frac{\partial T}{\partial x}\right|_{x=1}$$

- Heat transfer equation,
  – boundary temperature input *u*
  – heat flux output *y*
- Pulse response and step response



Time



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