1.021, 3.021, 10.333, 22.00 Introduction to Modeling and Simulation
Spring 2011

Introduction

Lecture 1

Markus J. Buehler

Laboratory for Atomistic and Molecular Mechanics
Department of Civil and Environmental Engineering
Massachusetts Institute of Technology

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**.

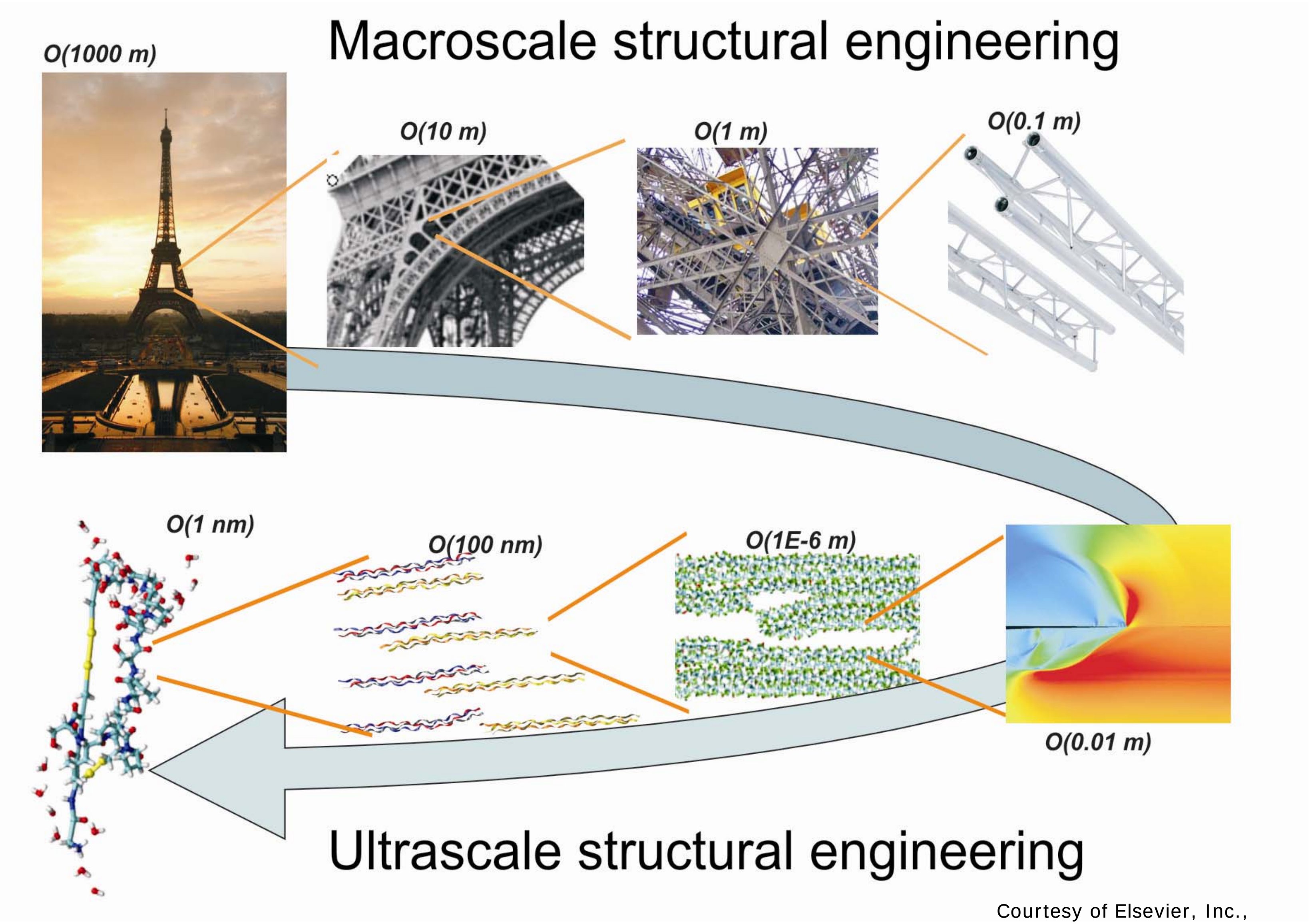
- Scientists and engineers have long used **models to better understand the system they study, for analysis and quantification, performance prediction and design**. However, in recent years – due to the advance of computational power, new theories (Density Functional Theory, reactive force fields e.g. 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



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Buehler and Ackbarow, *Materials Today*, 2007

Characteristic scale of **technology frontier** (materials)

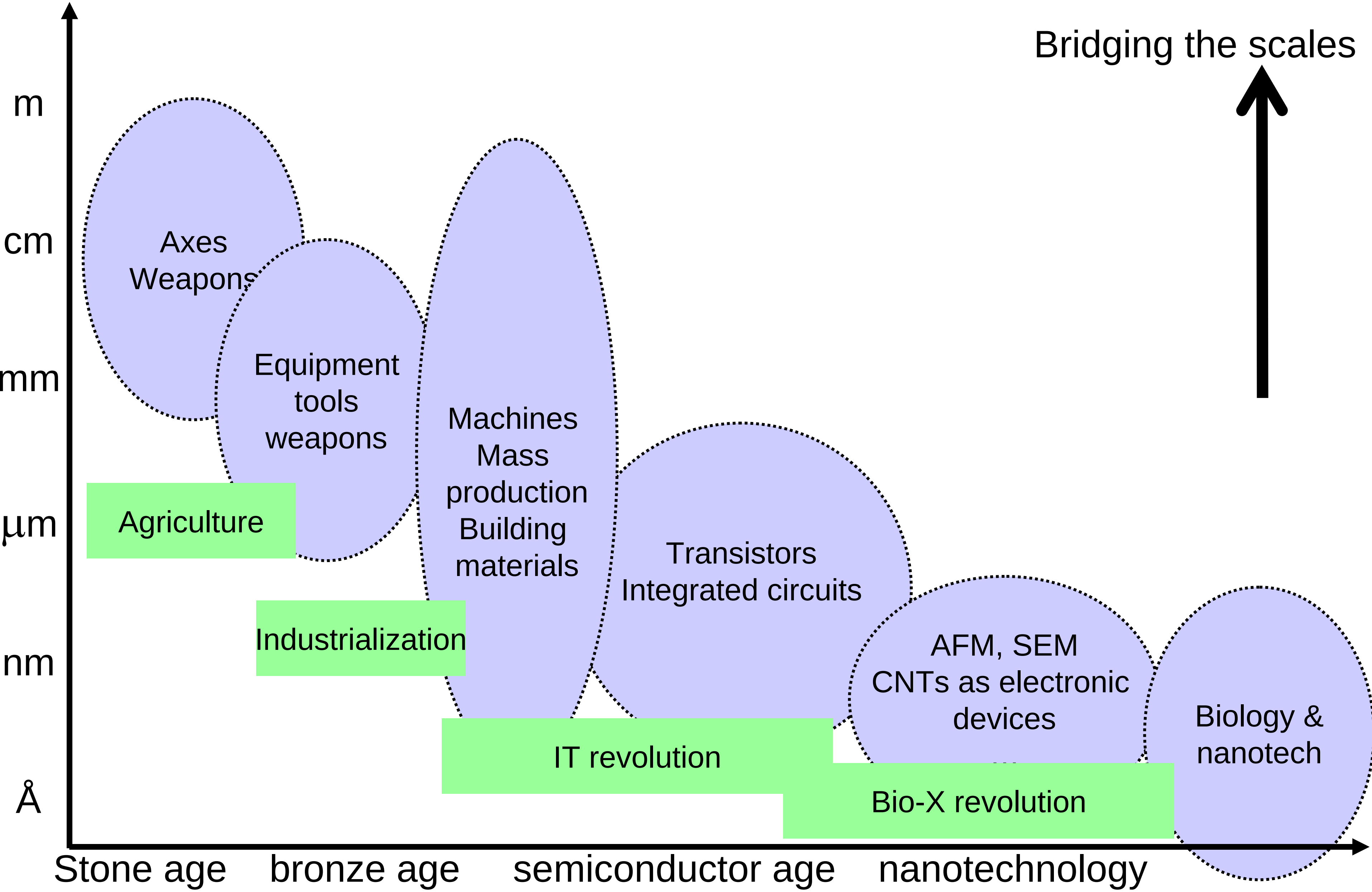


Fig. 1.1 in Buehler, Markus J. *Atomistic Modeling of Materials Failure*. Springer, 2008.

Content overview

I. Particle and continuum methods

Lectures 1-13

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

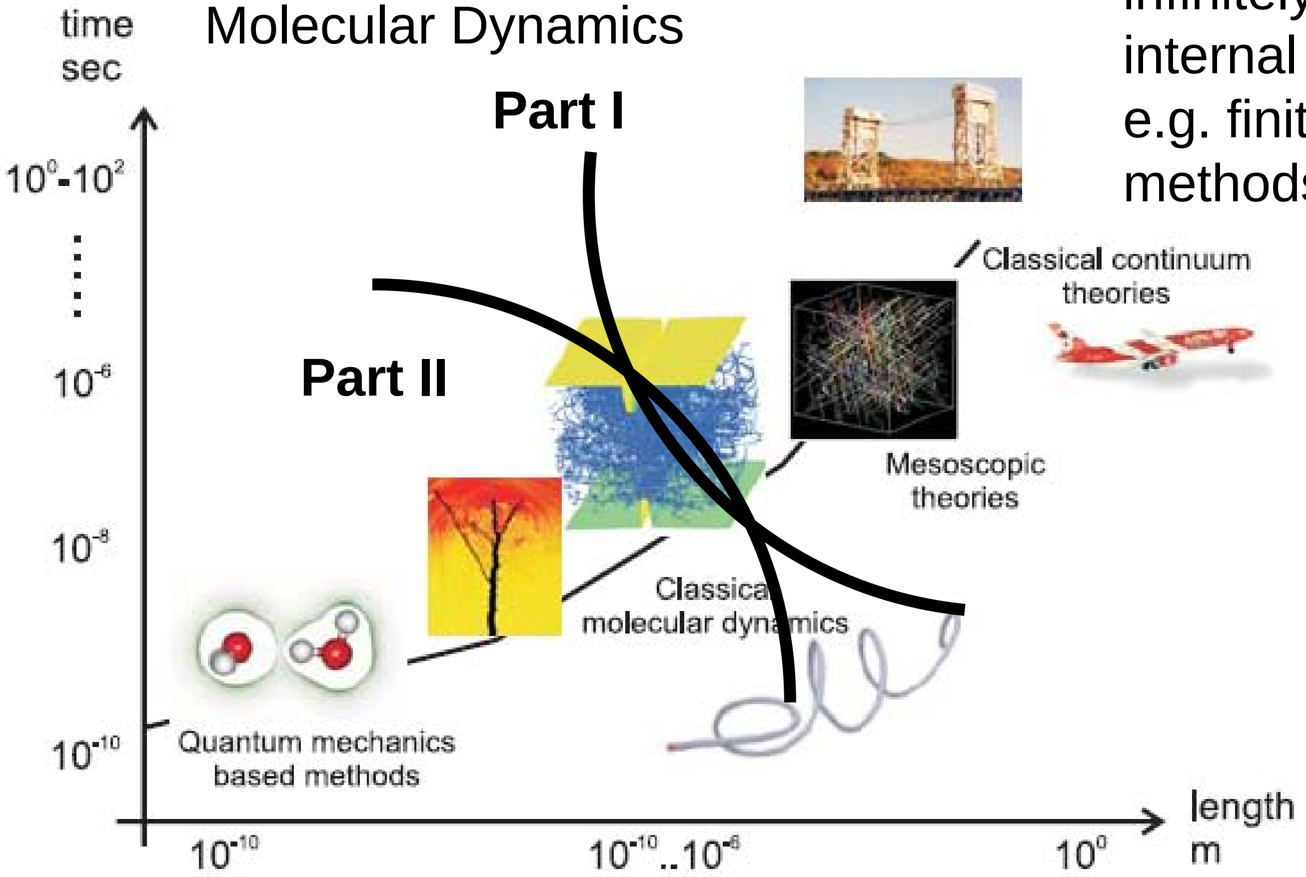
Lectures 14-26

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?

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

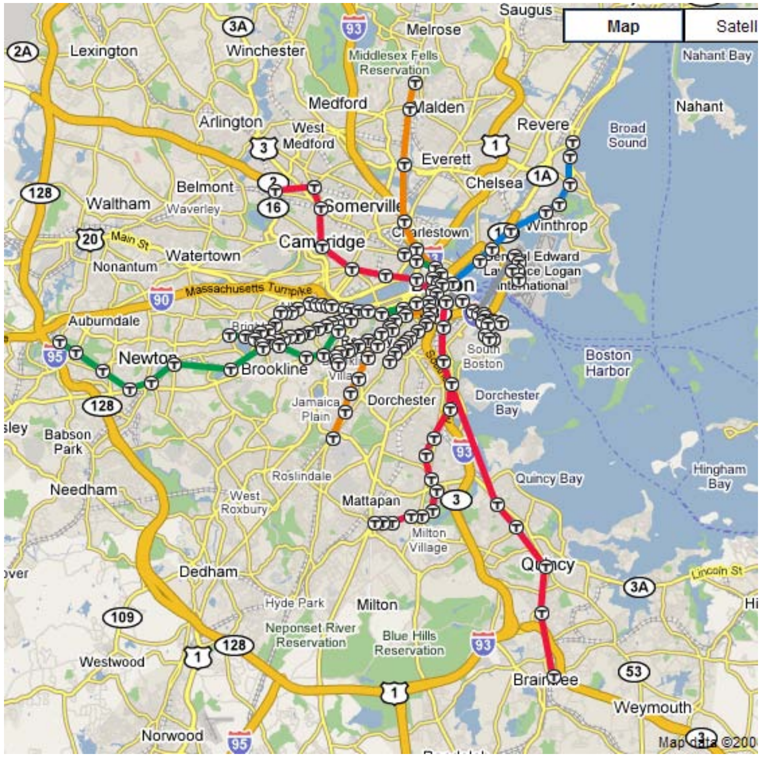
- The term *modeling* refers to the development of a mathematical representation of a physical situation.

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

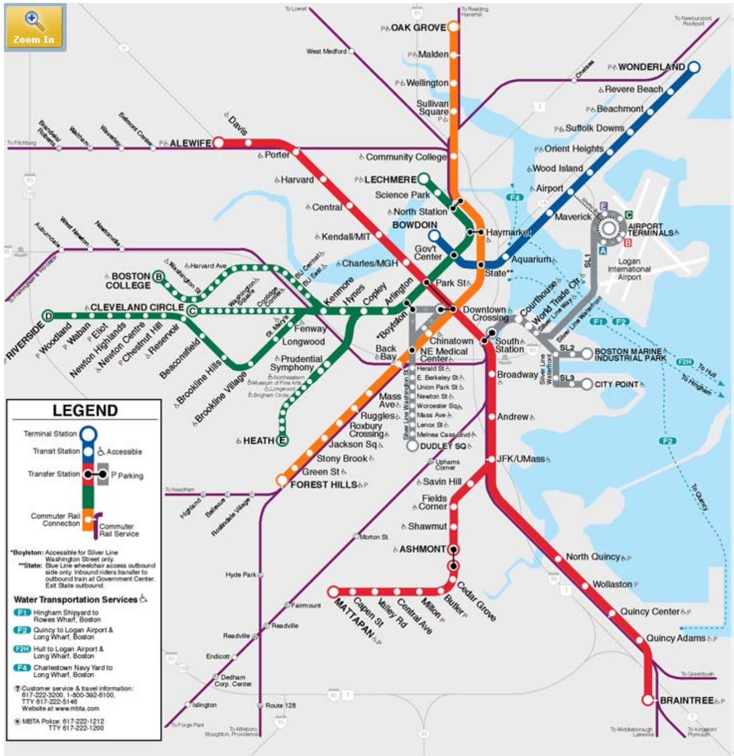
What is a model?

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.*



"Physical situation"



"Model"

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?

- 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.

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

+ BCs, ICs

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Part I – Continuum and particle methods

Introduction part I

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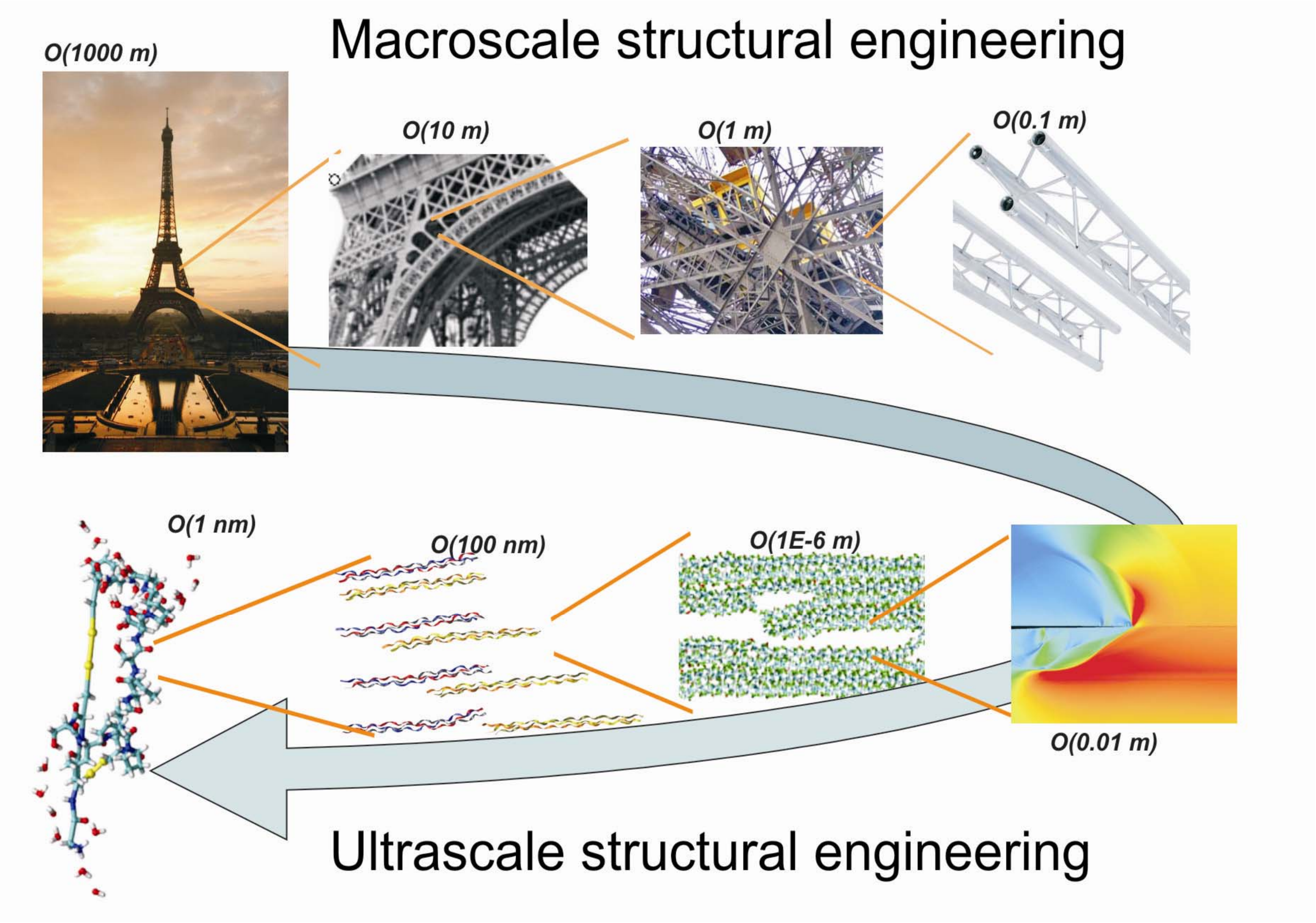
Multi-scale view of materials



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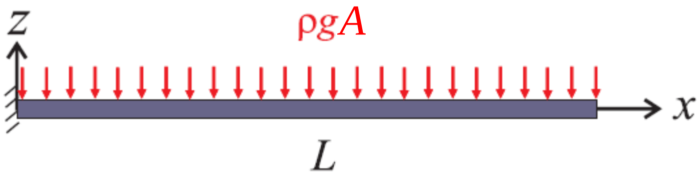
Buehler and Ackbarow, *Materials Today*, 2007

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



Question: Displacement field

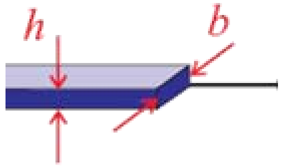
Governing equation (PDE)

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

Integration & BCs

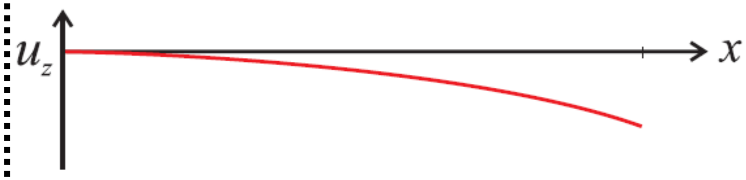
Geometry

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



BC - load:

$$\rho g A$$



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

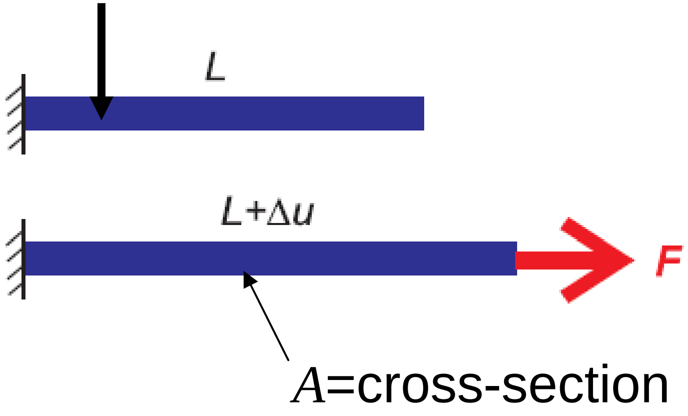
E = unknown parameter

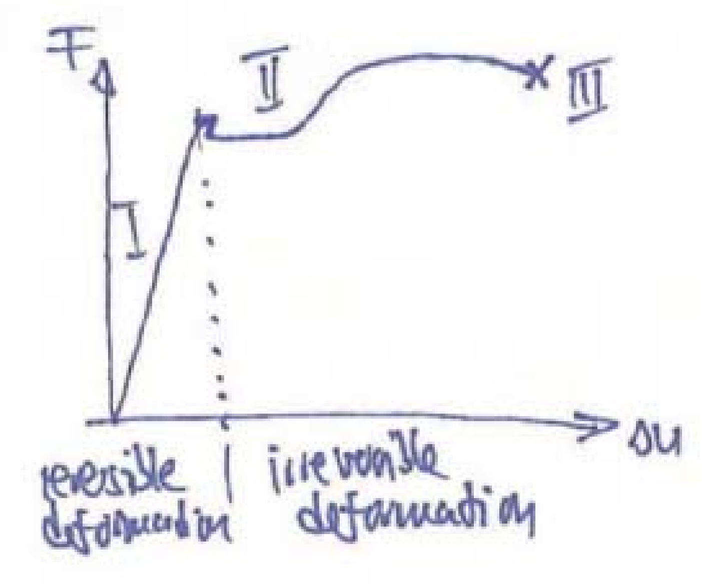
E is parameter called “Young’s modulus” that relates how force and deformation are related (captures properties of material)

How to determine Young’s modulus E ?

Measurement (laboratory):

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





$$F = k_s \Delta u$$

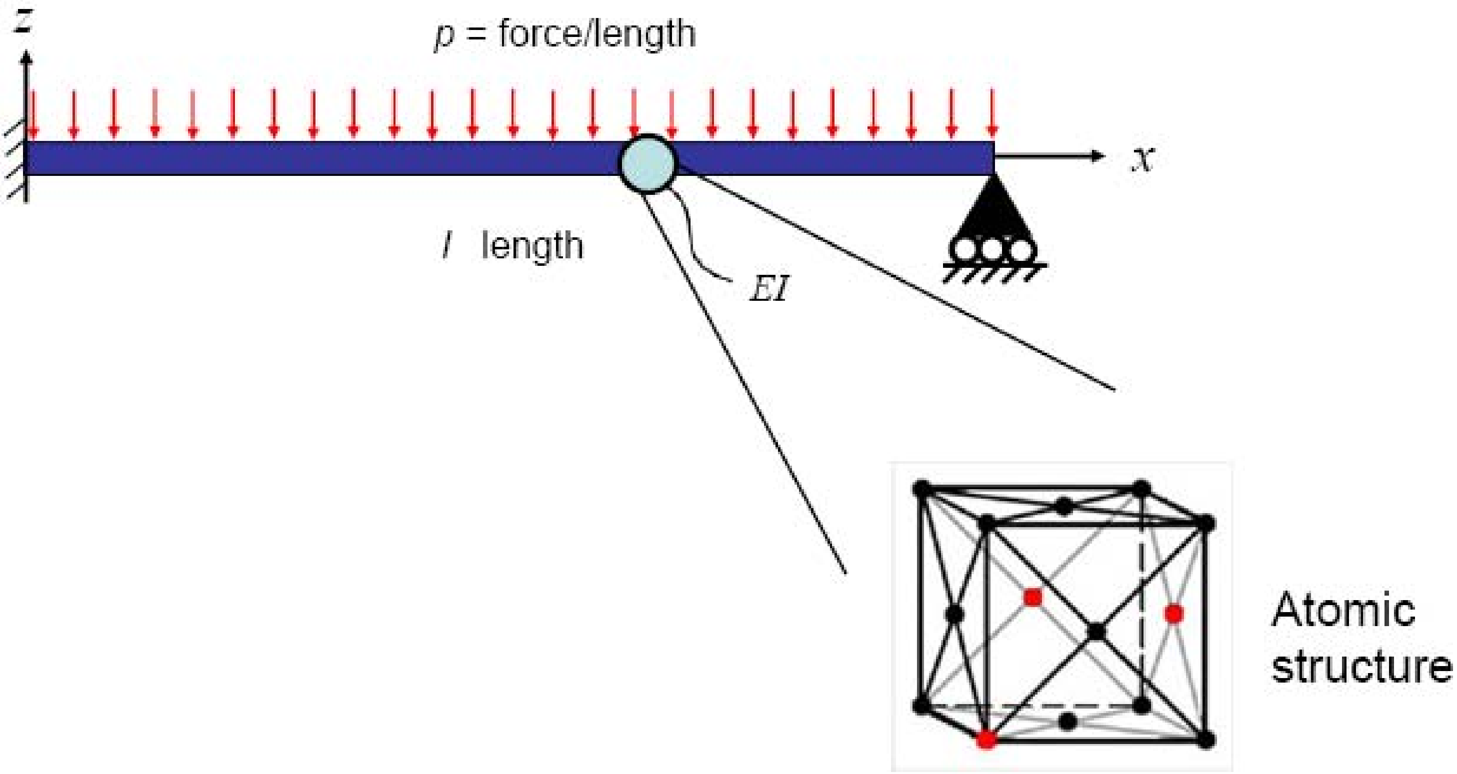
$$\downarrow$$

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

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

How to determine *E* ? - alternative approach

Atomistic simulation – *new engineering paradigm*



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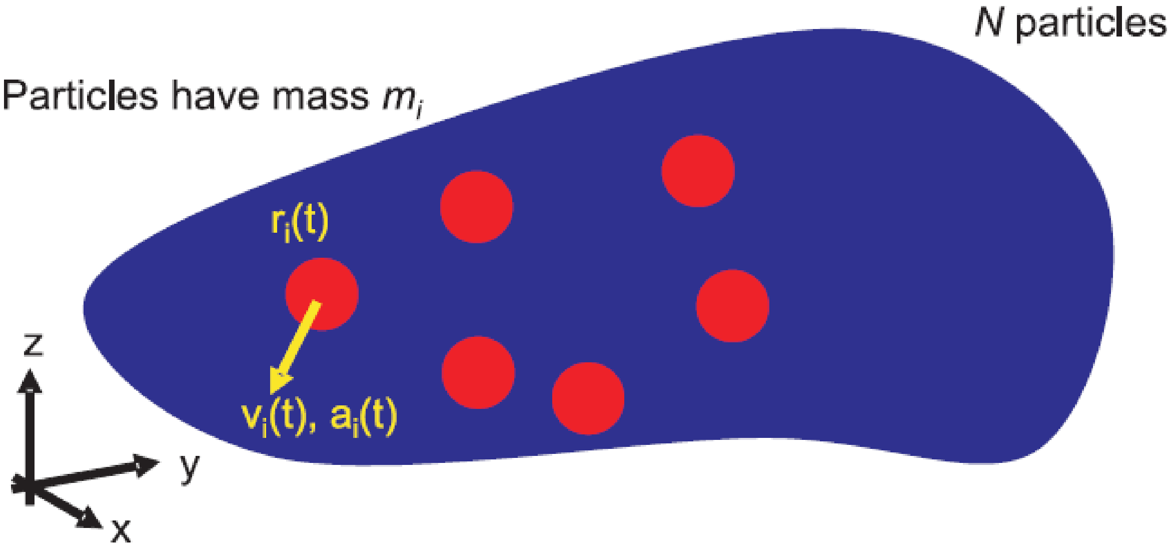
Idea: Consider the behavior of a collection of atoms inside the beam as deformation proceeds

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…)

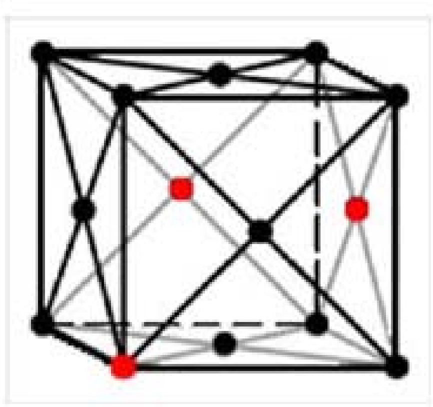


Linking atomistic and continuum perspective

- 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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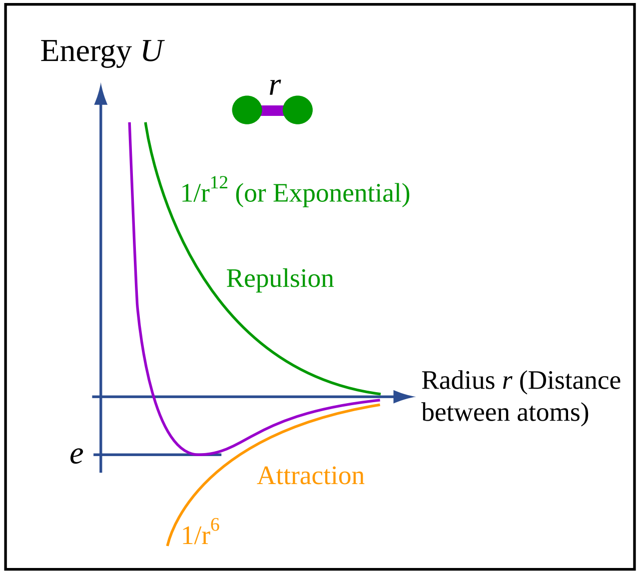

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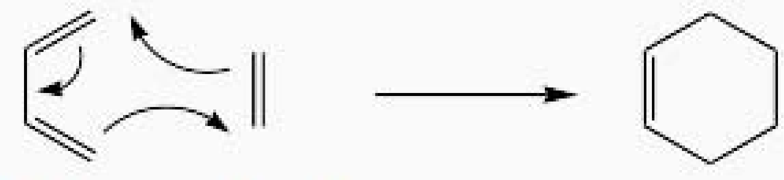
Quantum mechanics

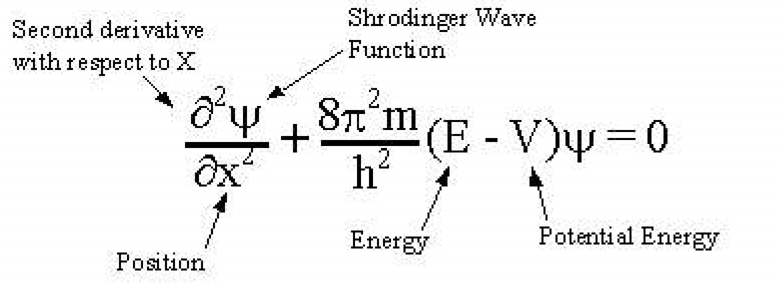
- Deals with fundamental view of chemical bonding, based on electrons in atoms



diene + dienophile

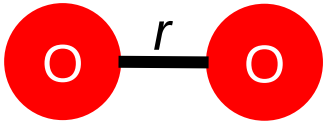
conjugated (substituted) diene + (substituted) olefin → (substituted) cyclohexene

“Schroedinger equation”



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

Developing a potential energy from quantum mechanics



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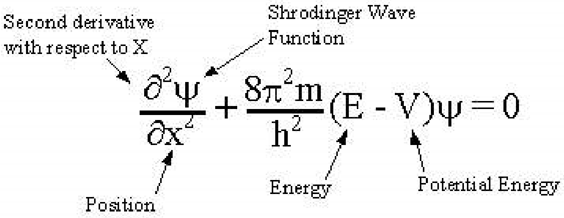
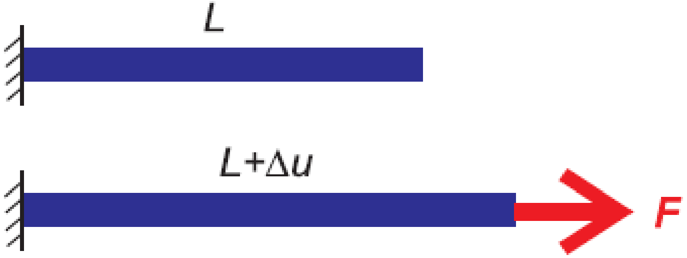


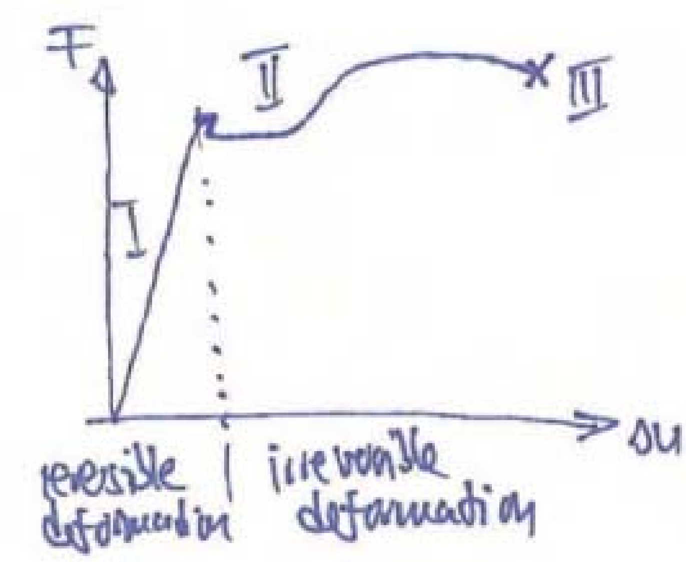
$$\frac{\partial^2\psi}{\partial x^2} + \frac{8\pi^2 m}{h^2}(E - V)\psi = 0$$

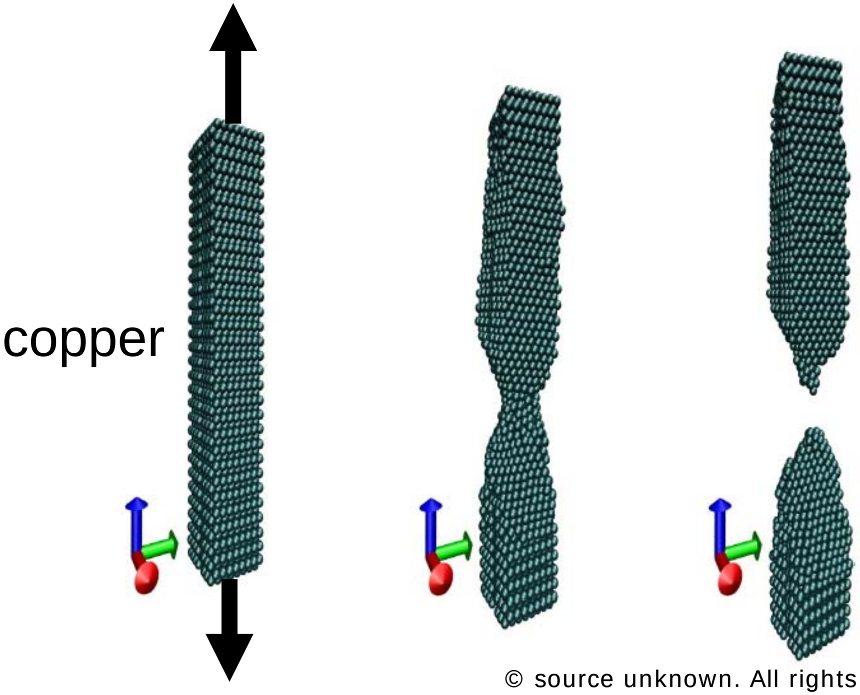
JAVA Applet

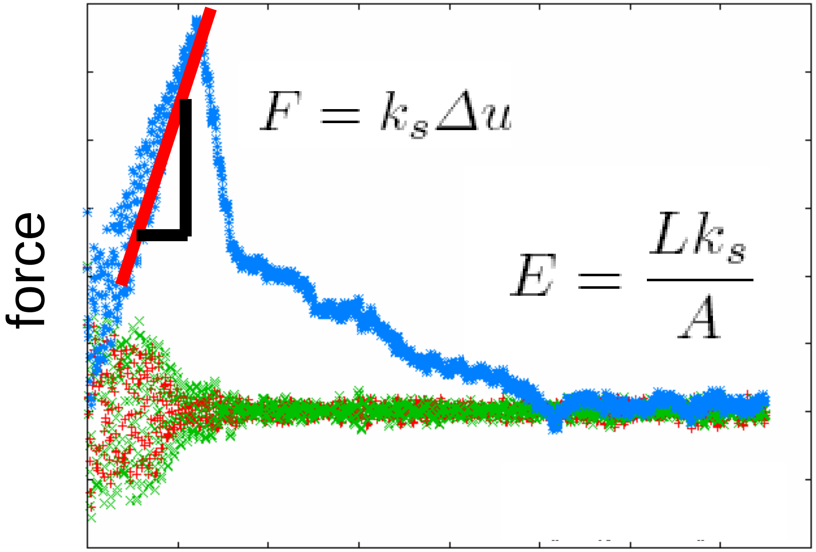
- http://webphysics.davidson.edu/WebTalks/AAPT_CISE_2000/Molecular/intro.html

Example: Stretching nanowire

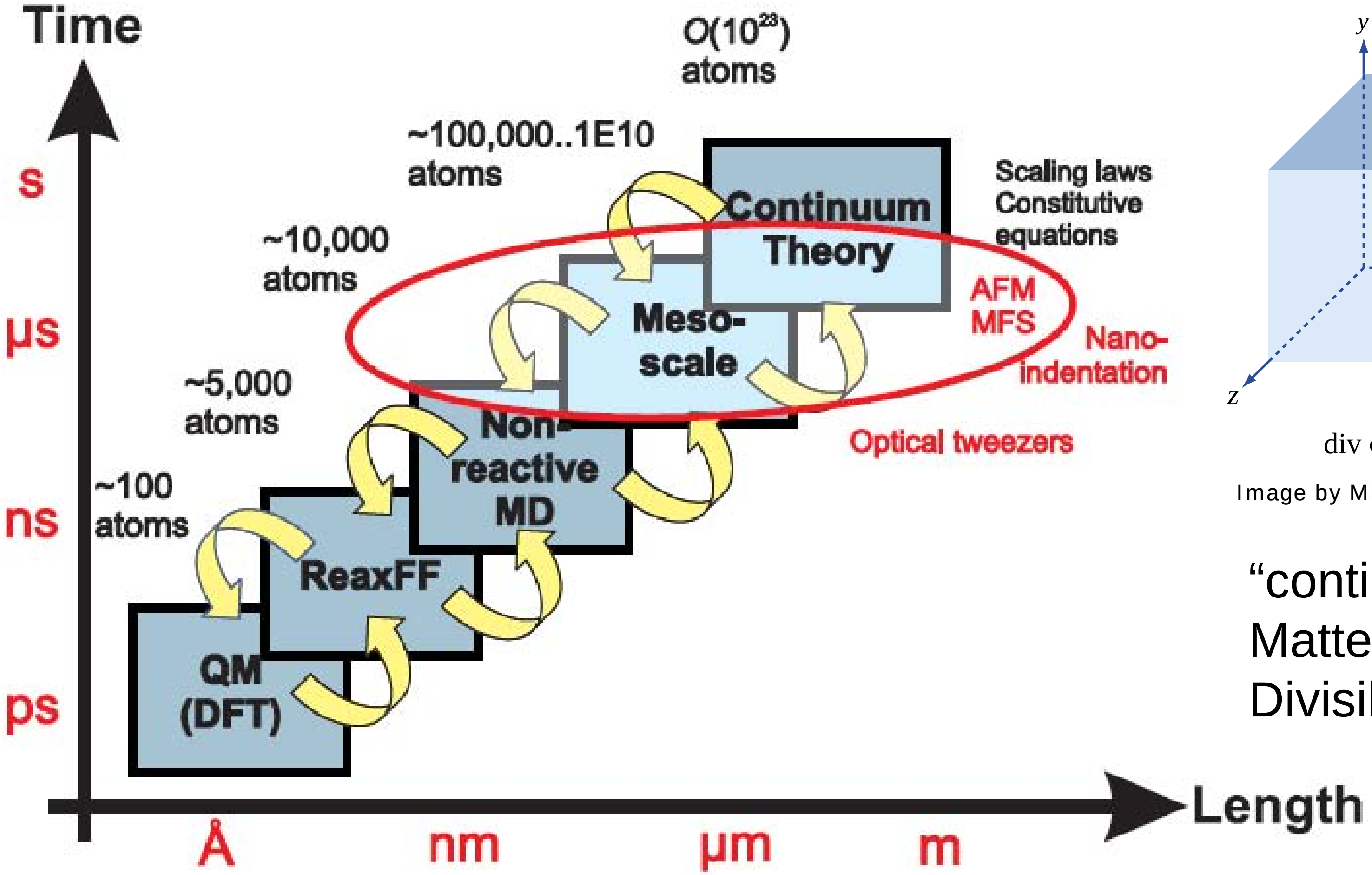


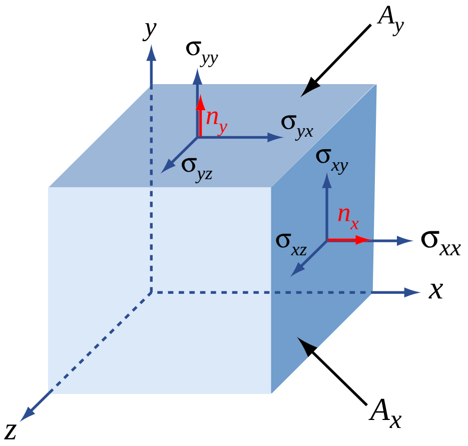






Multi-scale simulation paradigm





$$\operatorname{div} \sigma + f = 0$$

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"continuum scale"
Matter is indefinitely
Divisible

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

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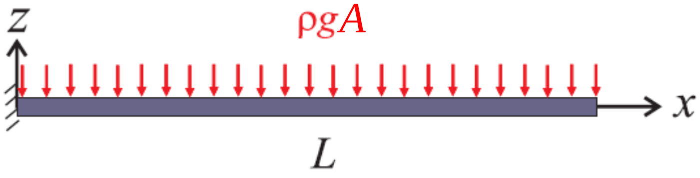
Beam deformation problem – continuum model



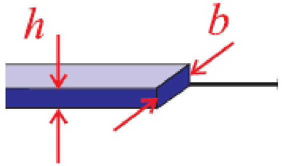
Question: Displacement field

Governing equation (PDE)

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

Geometry

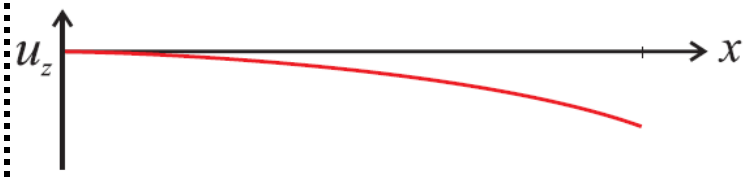
$$I_{zz} = \frac{bh^3}{12}$$



Integration & BCs

BC - load:

$$\rho g A$$



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

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

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Aivazis, Lombeyda and RR, 2003

Airbag deployment dynamics

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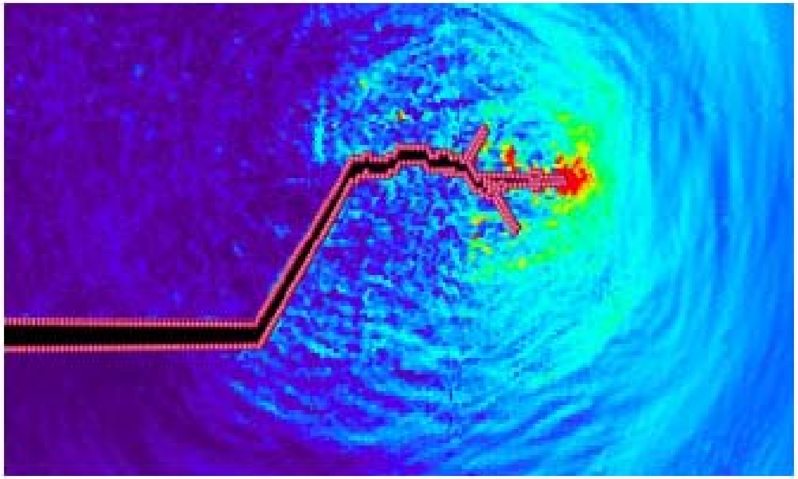
Benefits of atomistic models

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

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Public domain image.

Collapse of buildings

Image by quinn.anya on Flickr. License: CC-BY.

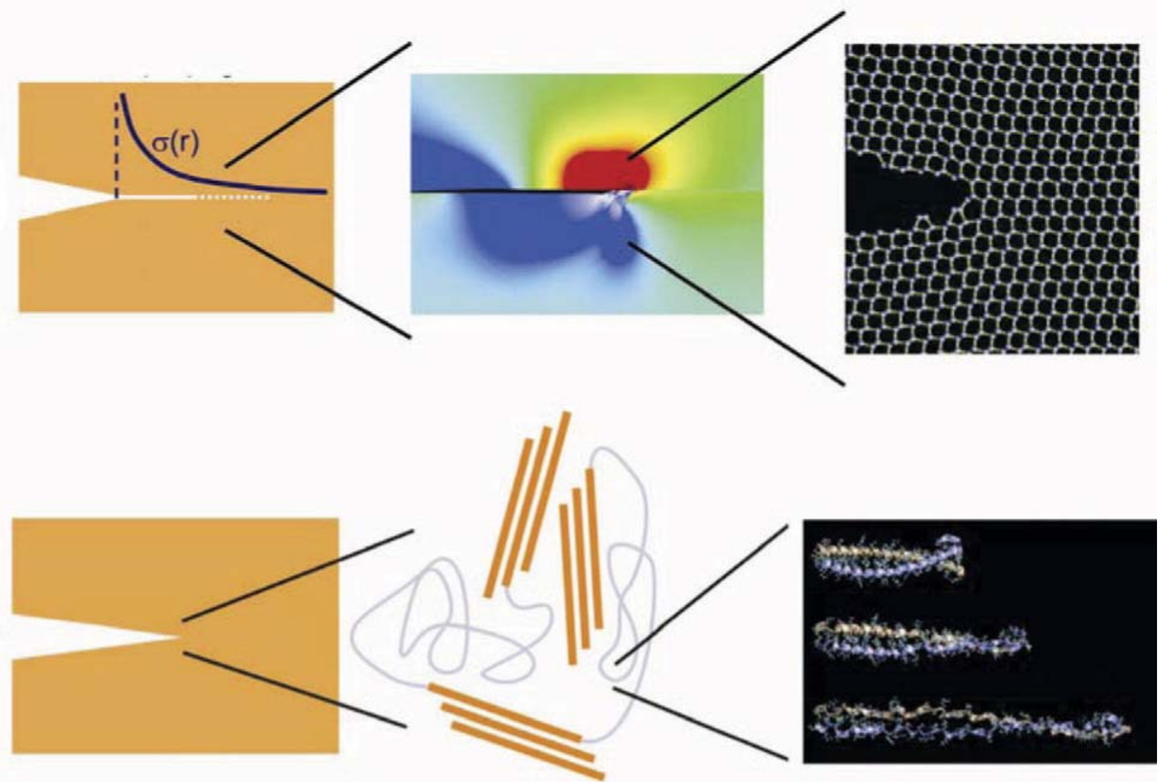
Engineering materials fracture (ceramics, tiles)

Bone fracture

Image by Wha'ppen on Flickr.

Cost of failure of materials: >>$100 billion (1982)

Failure proceeds by rupture and tear of molecular and atomistic structures



Breaking of chemical bonds

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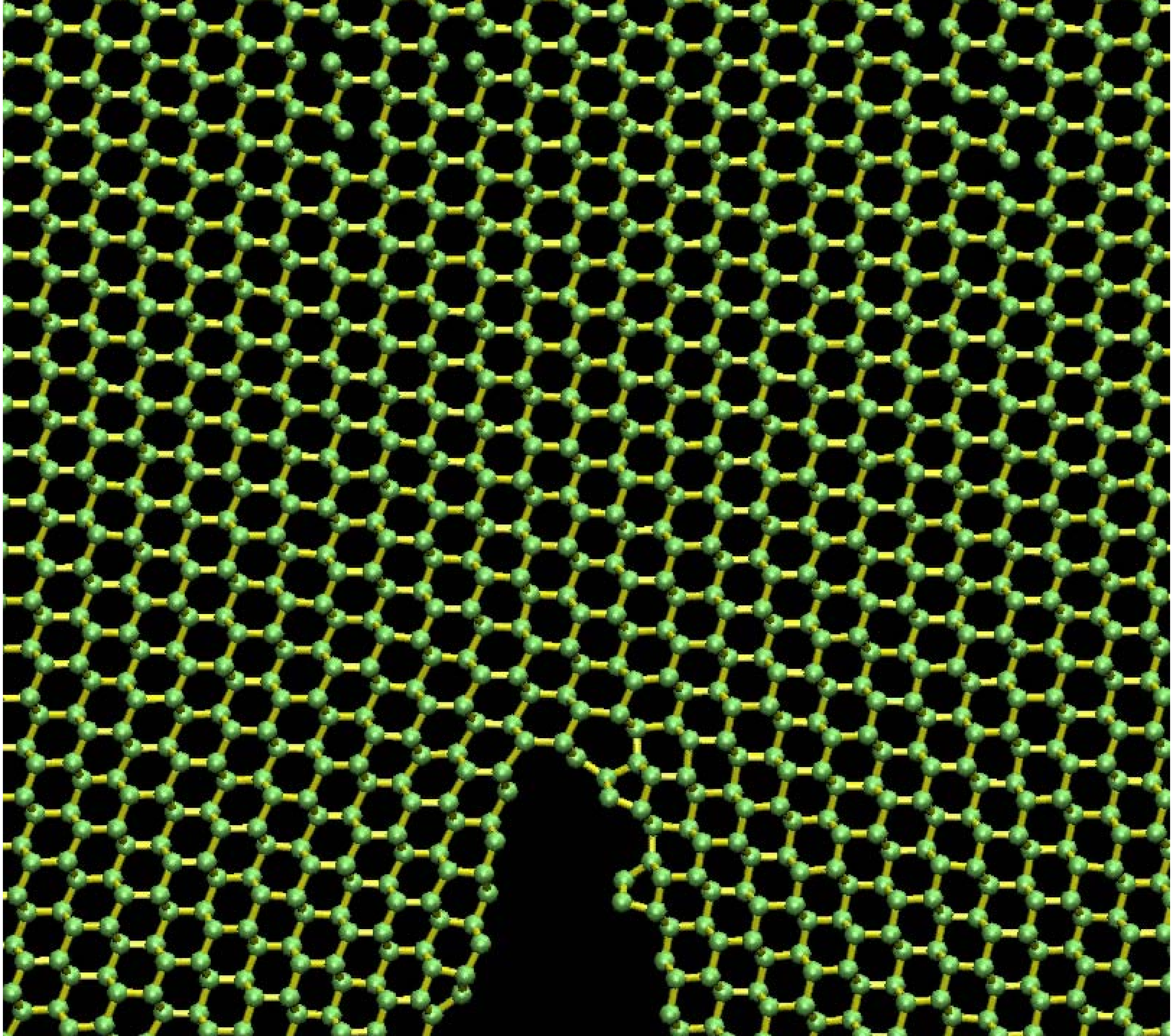
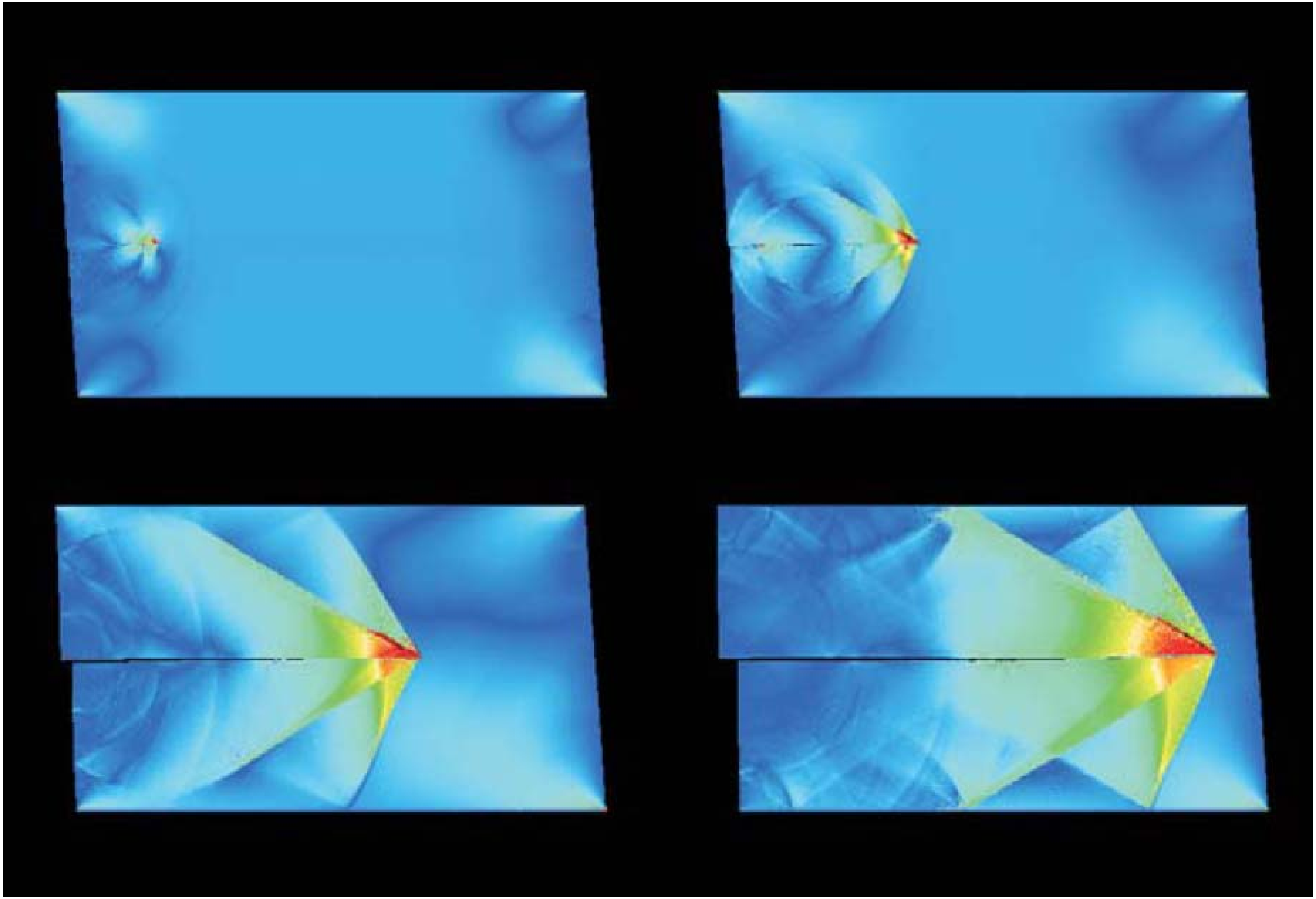
Failure of materials observed at macroscale is due to repeated breaking, shearing, tearing of bonds at atomistic scale

Nanoscopic response of material's building block is key for materials failure



http://web.mit.edu/mbuehler/www/research/supersonic_fracture.mpeg



Please see: Buehler, Markus J., Farid F. Abraham, et al. "Hyperelasticity Governs Dynamic Fracture at a Critical Length Scale." *Nature* 426 (2003): 141-6.

Supersonic fracture: Discovered in atomistic simulation on supercomputers

Theory/MD

experiment

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Please see Fig. 9 in Buehler, Markus, and Huajian Gao. "Modeling Dynamic Fracture Using Large-Scale Atomistic Simulations." Chapter 1 in Shukla, Arun. *Dynamic Fracture Mechanics*.Hackensack, NJ: World Scientific, 2006.

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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

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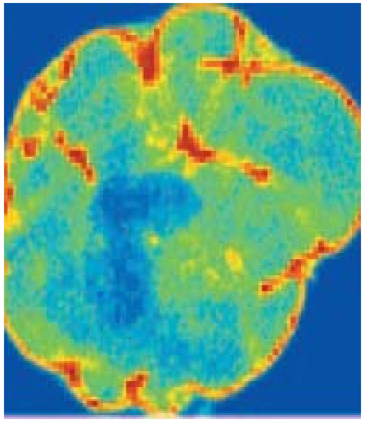
→

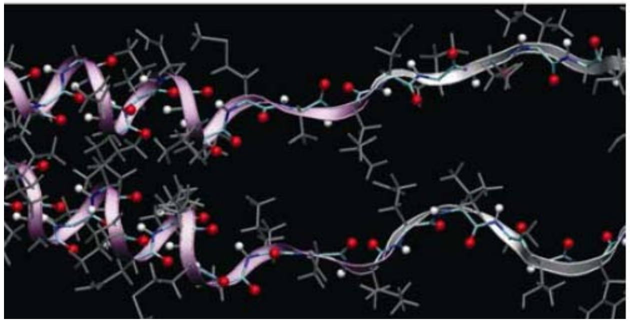
Fracture in cell's nucleus
Created under mechanical deformation



Reprinted by permission from Macmillan Publishers Ltd: *Nature Materials.*
Source: Buehler, M., and Y. Yung. "Deformation and Failure of Protein Materials in Physiologically Extreme Conditions and Disease." *Nature Materials* 8, no. 3 (2009): 175-88. © 2009.

→

Failure of protein molecules
Building blocks of life



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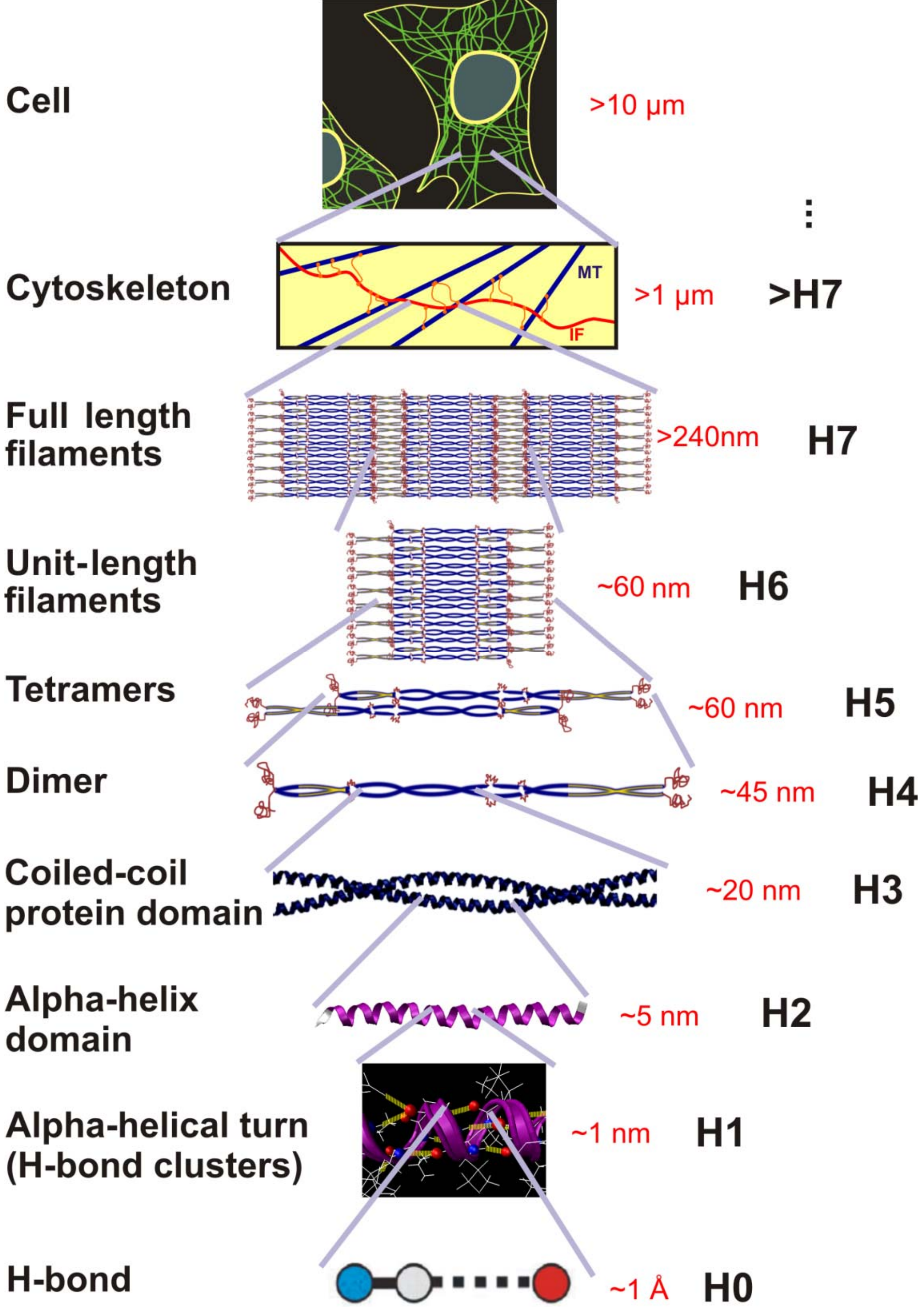
Vimentin intermediate filament

Cells

Filaments

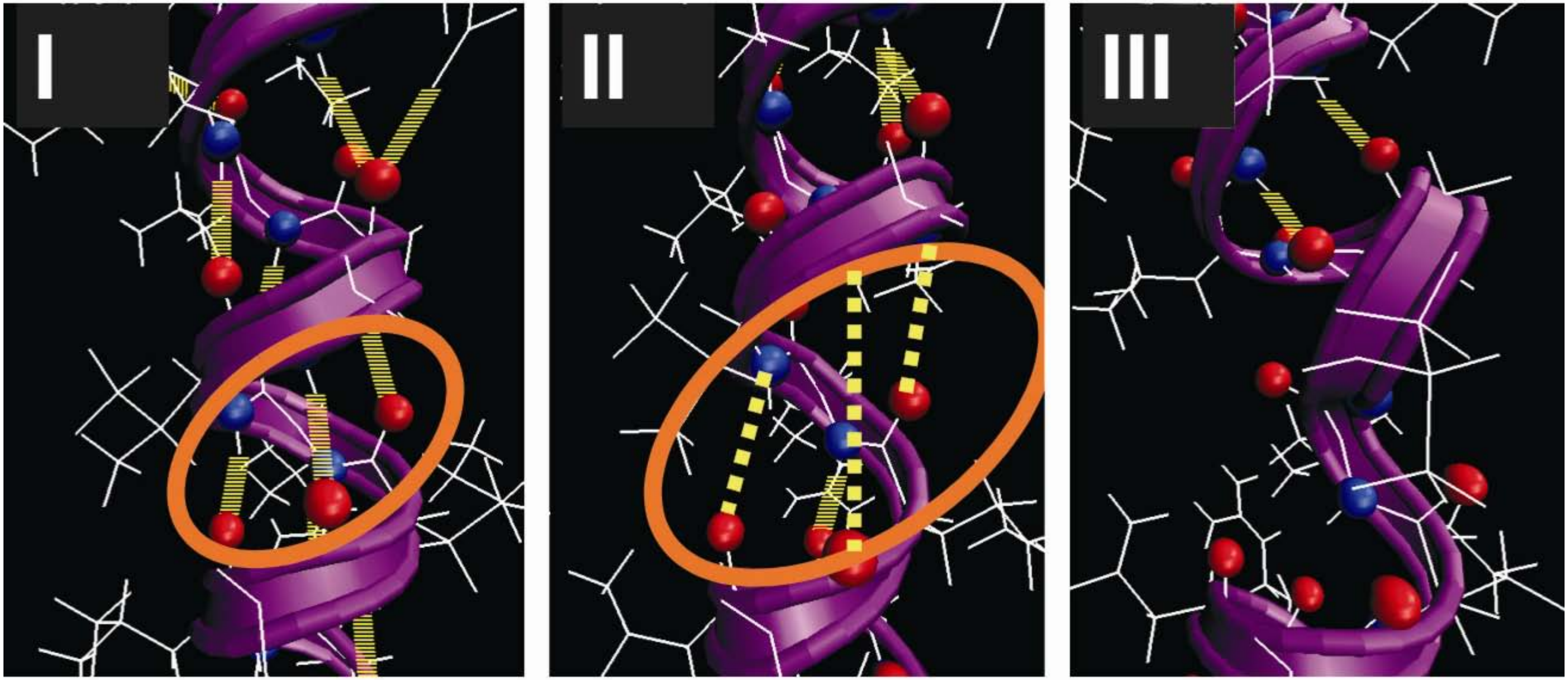
Protein molecule

Chemical bonding



Source: Qin, Z., L. Kreplak, and M. Buehler. "Hierarchical Structure Controls Nanomechanical Properties of Vimentin Intermediate Filaments." *PLoSONE* 4, no. 10 (2009). doi:10.1371/journal.pone.0007294. License CC BY.

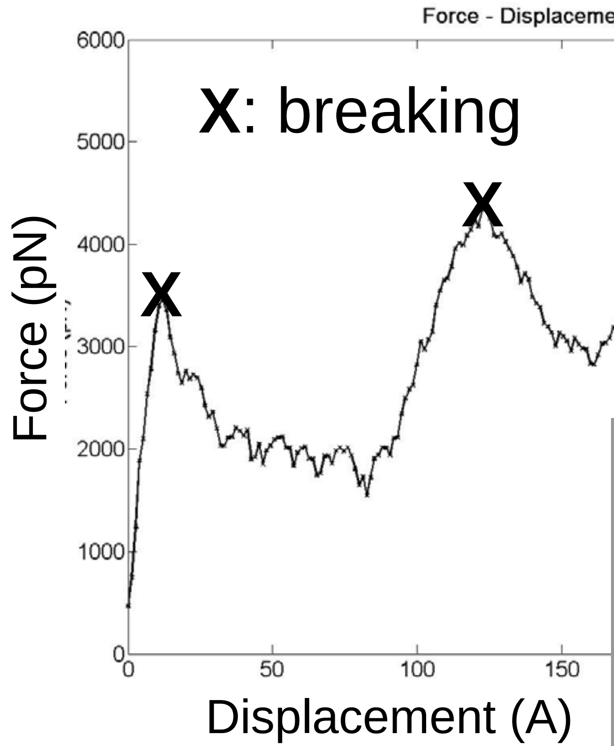
How structural building blocks of cells break



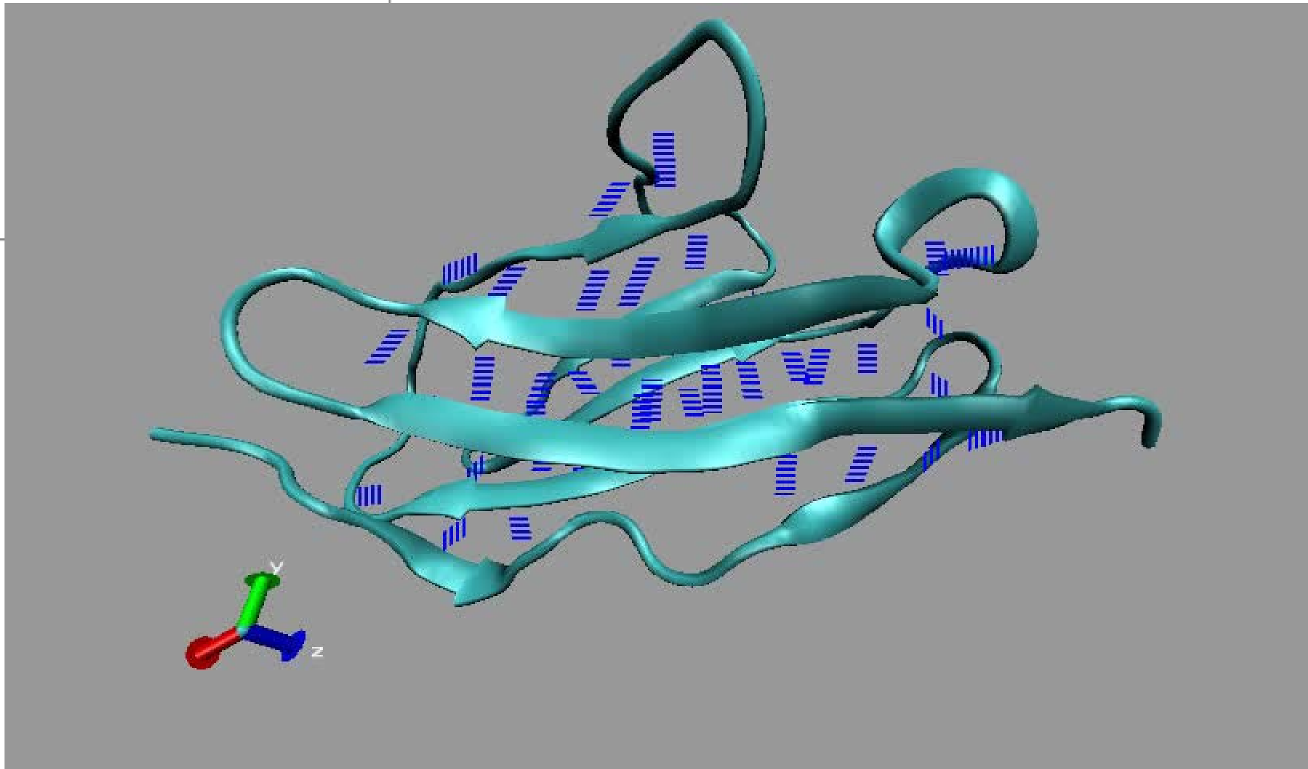
Courtesy of National Academy of Sciences, U. S. A. Used with permission.
Source: Ackbarow, Theodor, et al. "Hierarchies, Multiple Energy Barriers, and Robustness Govern the Fracture Mechanics of Alpha-Helical and Beta-Sheet Protein Domains." *PNAS* 104 (2007): 16410-15. Copyright 2007 National Academy of Sciences, U.S.A.

- Genetic diseases
- Molecular **mechanisms** of biology

Unfolding of titin molecule

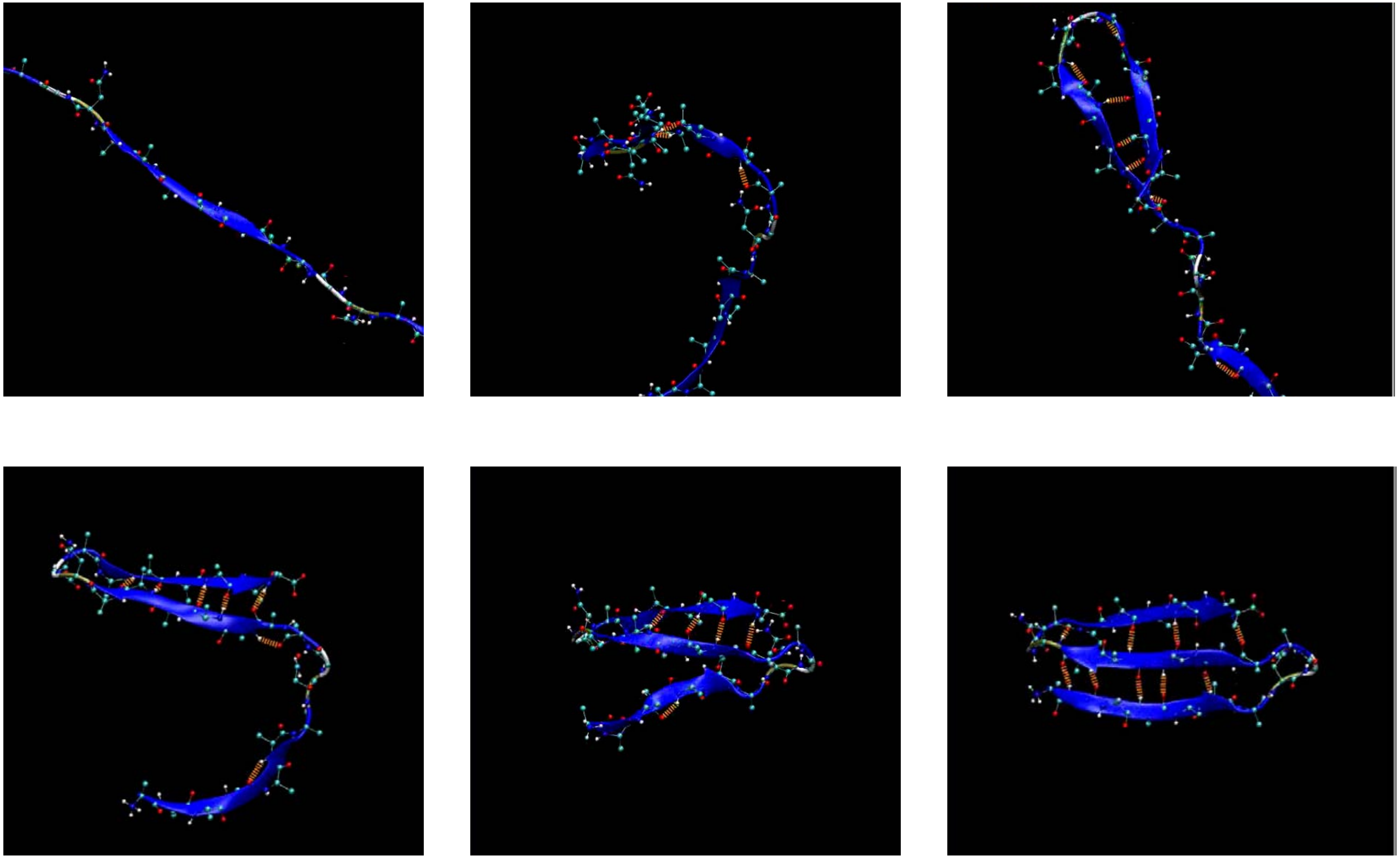


Titin I27 domain: Very resistant to unfolding due to parallel H-bonded strands

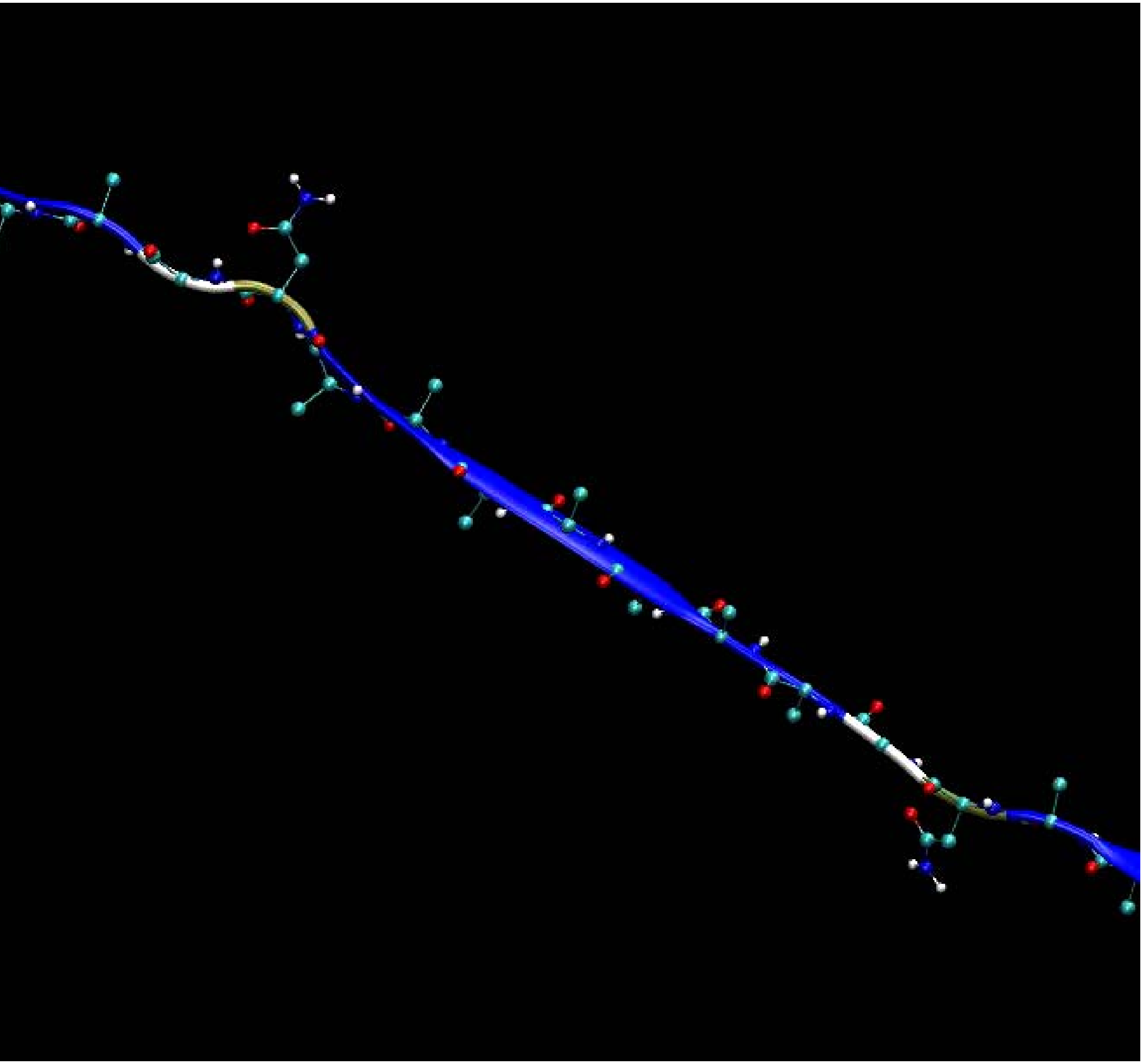


Keten and Buehler, 2007

Folding of beta-sheet protein structure



Movie



S. Keten and M.J. Buehler, *in submission*

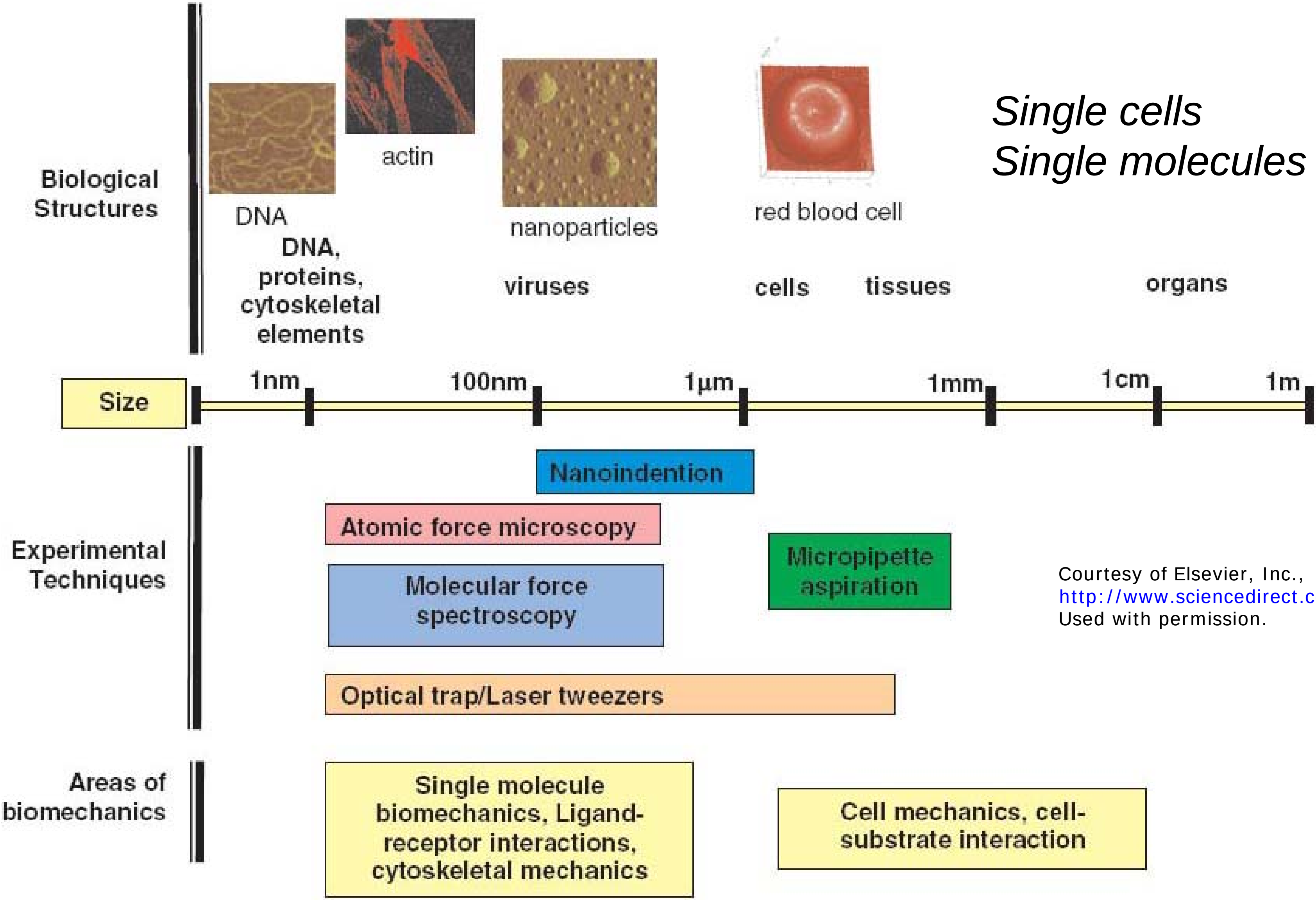
A New Approach to Molecular Simulation

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

Folding@home distributed computing

http://folding.stanford.edu/

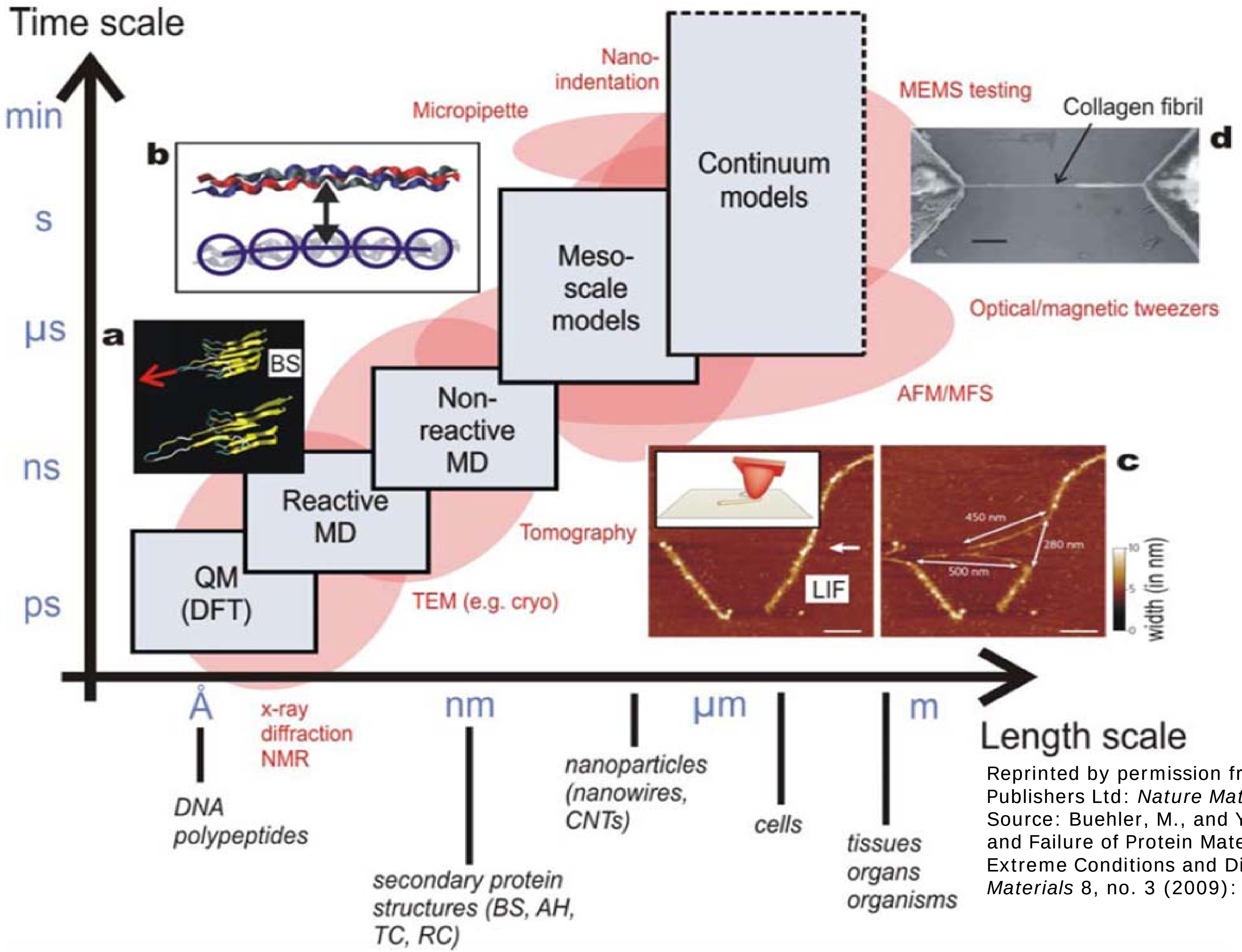
Opportunity: Experimental techniques



Single cells
Single molecules

Courtesy of Elsevier, Inc., http://www.sciencedirect.com. Used with permission.

Integration with experimental techniques



Reprinted by permission from Macmillan Publishers Ltd: *Nature Materials.*
Source: Buehler, M., and Y. Yung. "Deformation and Failure of Protein Materials in Physiologically Extreme Conditions and Disease." *Nature Materials* 8, no. 3 (2009): 175-88. © 2009.

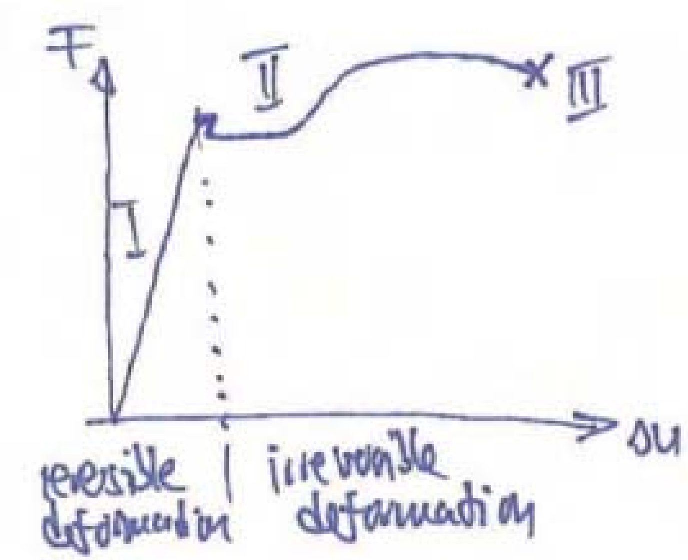
For most applications, we will use a website-driven simulation framework developed in collaboration with MIT’s Office for Undergraduate Education

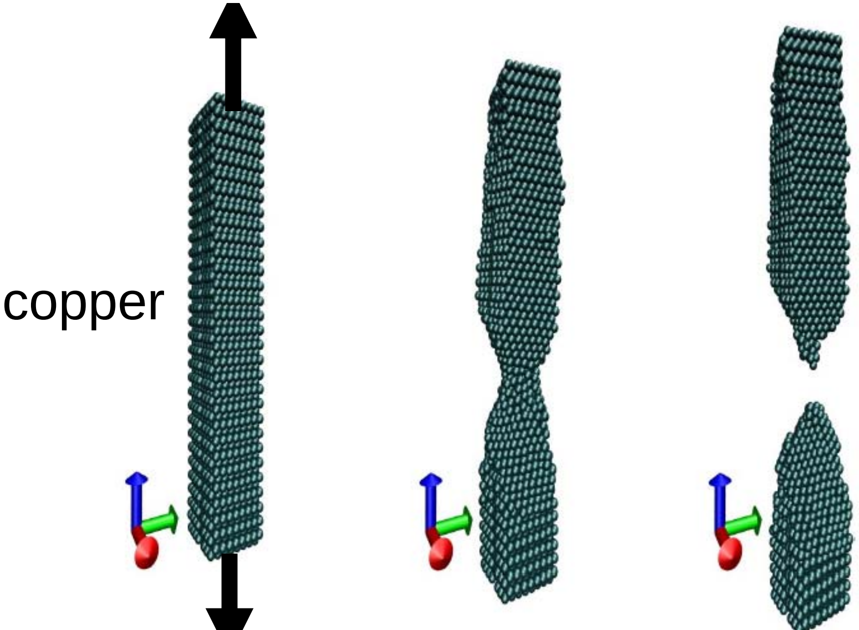
nanoHUB: https://nanohub.org

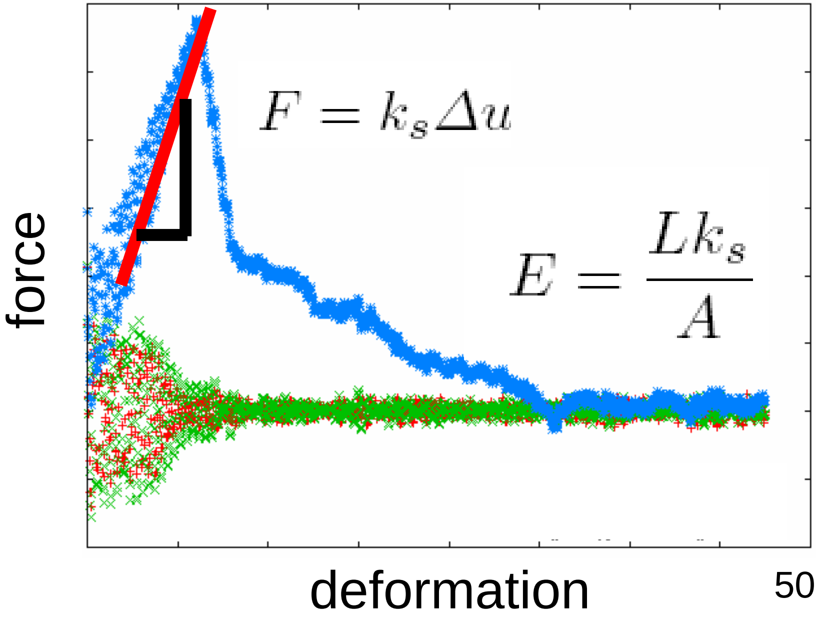
More than 160 tools:
https://nanohub.org/resources/tools

Technical assistance: Justin Riley

Example: Stretching nanowire







3.021J / 1.021J / 10.333J / 18.361J / 22.00J Introduction to Modeling and Simulation
Spring 2012