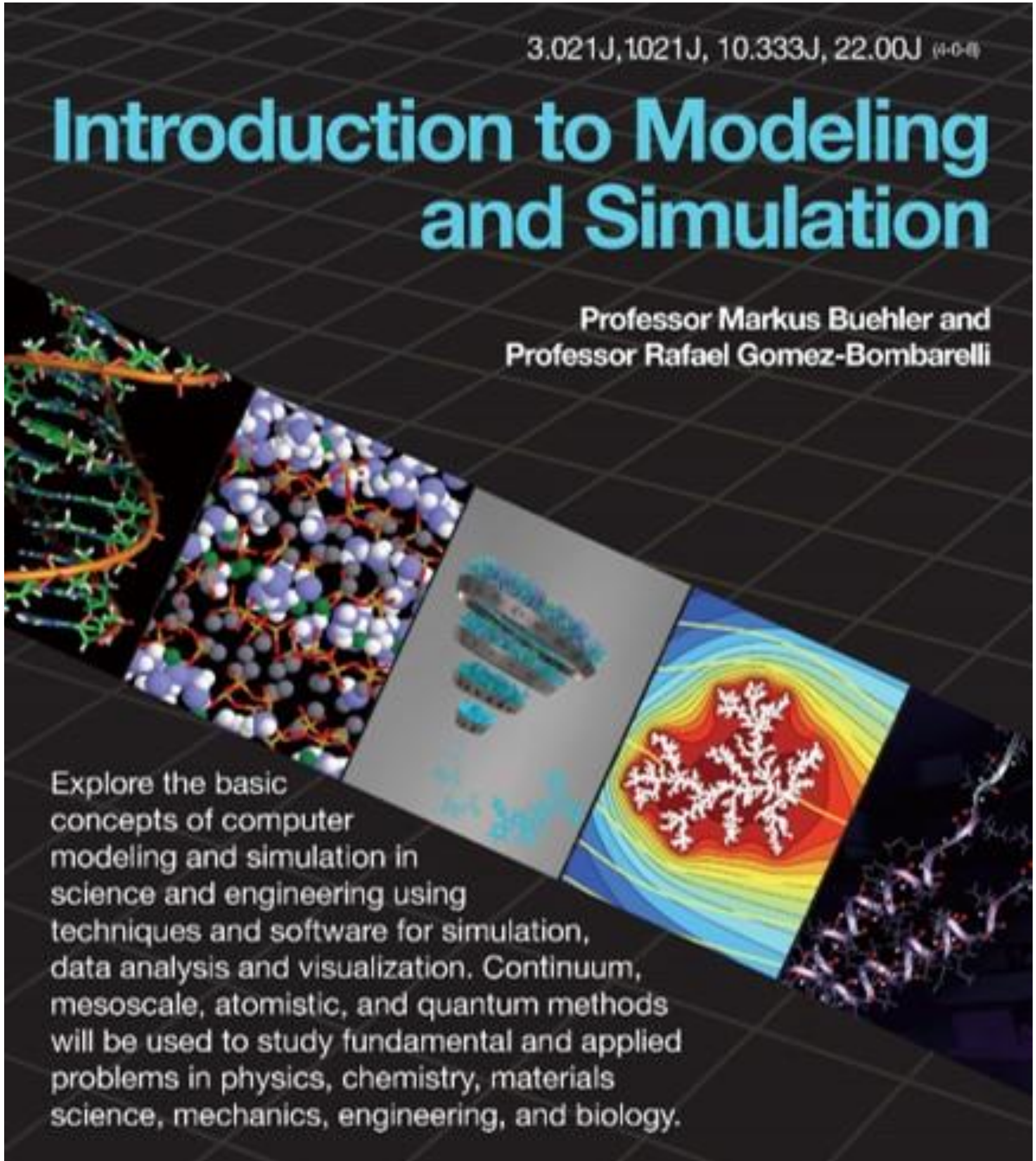

3.021J, 1021J, 10.333J, 22.00J
Introduction to Modeling and Simulation
Professor Markus Buehler and
Professor Rafael Gomez-Bombarelli
Explore the basic concepts of computer modeling and simulation in science and engineering using techniques and software for simulation, data analysis and visualization. Continuum, mesoscale, atomistic, and quantum methods will be used to study fundamental and applied problems in physics, chemistry, materials science, mechanics, engineering, and biology.

1.021, 3.021, 10.333, 22.00 Introduction to Modeling and Simulation
Spring 2018

Introduction

Lecture 1

Instructors: Markus J. Buehler & Rafael Gomez-Bombarelli
Recitation instructor: Francisco Martinez

Massachusetts Institute of Technology

Welcome to Introduction to Modeling and Simulation!

Teaching team IM/S Spring 2018

Instructors:

- Markus J. Buehler (office 1-290, phone x2-2750, mbuehler@MIT.EDU)
  Department of Civil and Environmental Engineering

- Rafael Gomez-Bombarelli (office 13-5037, x3-5632, rafagb@mit.edu)
  Department of Materials Science and Engineering

- **Office hours:** Send an email to arrange a time

Recitation instructor:

- Francisco Martinez (office 1-235, fmartinm@mit.edu)
  Department of Civil and Environmental Engineering
  Office hours: TBA

Lectures:

- Two sessions per week TR 3-4:30 in 4-231

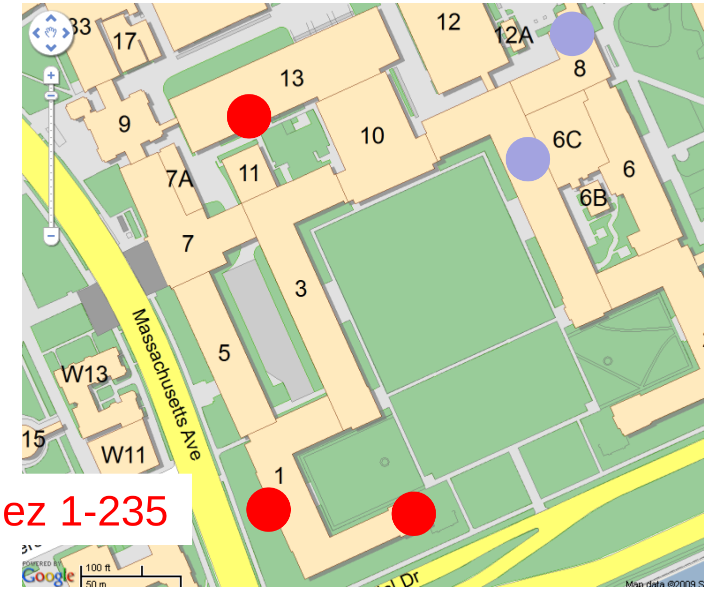
Recitations:

- Monday and Friday 4-5 pm in 8-205
  "Identical" versions of recitations given

Contact information

Lecture (4-231) &
recitation (8-205)

Rafael Gomez-Bombarelli 13-5037



Fran Martinez 1-235

Office Markus Buehler 1-290

Subject structure and grading scheme

Part I: Fundamentals of particle methods (Markus Buehler)
Lectures 1-13

Part II: Quantum mechanics (Rafael Gomez-Bombarelli)
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 in-class quizzes (50%)

Quizzes and final exam

- Each of the two parts will be followed by an in-class exam
- Duration 80 minutes
- Open book

Tentative dates:

- Quiz I (covers part I): Thursday, March 22, 2018
- Quiz II (covers part II): Thursday, May 10, 2018

The exams will cover simple calculations, theoretical material and important concepts (example questions given in review lecture prior to quiz)

Homework assignments

- Each part will contain approximately 2-3 problem sets with approximately 1-2 weeks preparation time.
- Problem sets can be solved in groups. Each group turns in one copy, with a statement required that each member of the team contributed actively. Groups must stay the same throughout the semester
- Due dates for problem sets are firm and homework assignments will be corrected and handed back (with solutions).
- You may use any material to complete the solution. However, it is important that you properly reference the material used (e.g. books, websites, scholarly journal articles, etc.).
- In Monday’s and Friday’s recitation we will discuss material relevant for the problem sets (solution approaches, computational methods,..) – attendance strongly encouraged.

Resources: Stellar class website

- https://stellar.mit.edu/S/course/1/sp18/1.021/index.html

- What will you find?
  - Logistics
  - Lecture notes
  - Assignments & solutions
  - Schedule, additional information, etc.
  - Reading material and reading assignments
  - Forum
  - Announcements (sent by instructors)

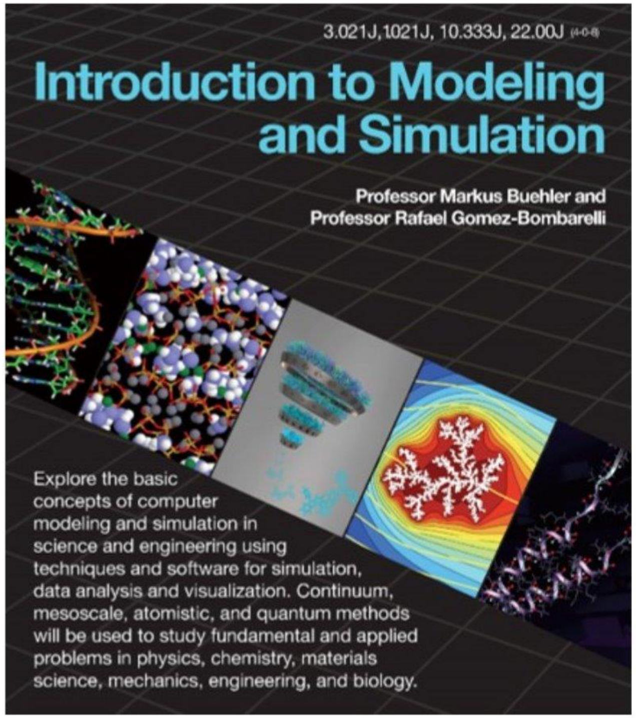
Class Home
Materials
Calendar
Homework
Gradebook Module
Forum

Membership
Staff List
Search
STELLAR HELP

Contact Help Desk

1.021/3.021/10.333/22.00 Intro to Modeling & Simulation

Spring 2018



Instructors: Markus J Buehler, Rafael Gomez-Bombarelli

TA: Francisco Martinez

Lecture: TR3-4.30 (4-231)
Recitation 1: M4-5 (8-205)
Recitation 2 : F4-5 (8-205)

Information:

Basic concepts of computer modeling and simulation in science and engineering. Uses techniques and software for simulation, data analysis and visualization. Continuum, mesoscale, atomistic and quantum methods used to study fundamental and applied problems in physics, chemistry, materials science, mechanics, engineering, and biology. Examples drawn from the disciplines above are used to understand or characterize complex structures and materials, and complement experimental observations.

Announcements

A few things we'd like you to remember…

- **We teach this class for you!** Our goal: **Discover the world of Modeling and Simulation with you** – using a bottom-up approach.

- Please let us know if you have concerns or suggestions, or if you have difficulties. We will do our best to maximize your learning experience.

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

- *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**.

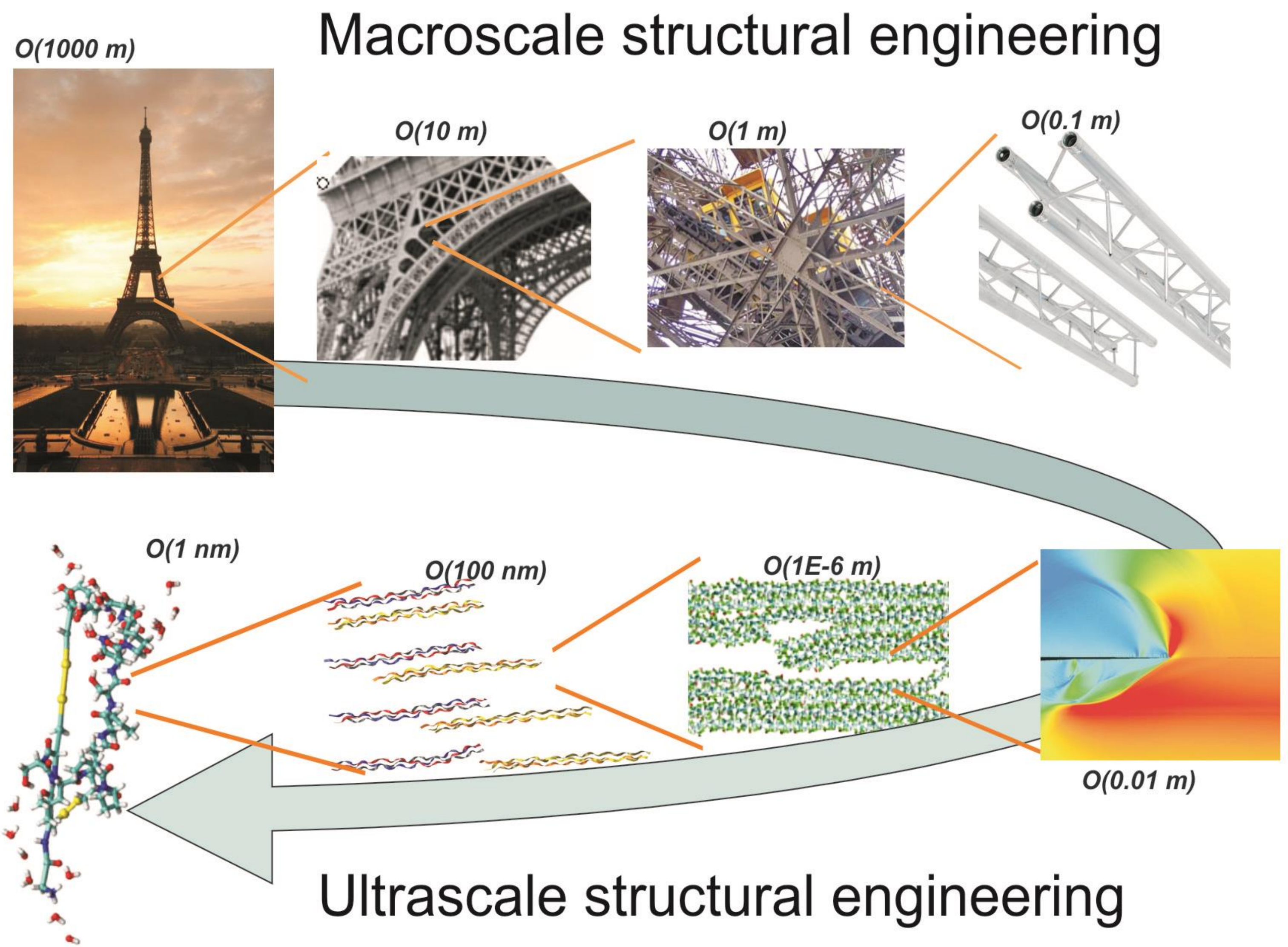
- Scientists and engineers have long used **models to better understand the system they study, for analysis and quantification, performance prediction and design**. However, in recent years – due to the advance of computational power, new theories (Density Functional Theory, reactive force fields e.g.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

- 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!***

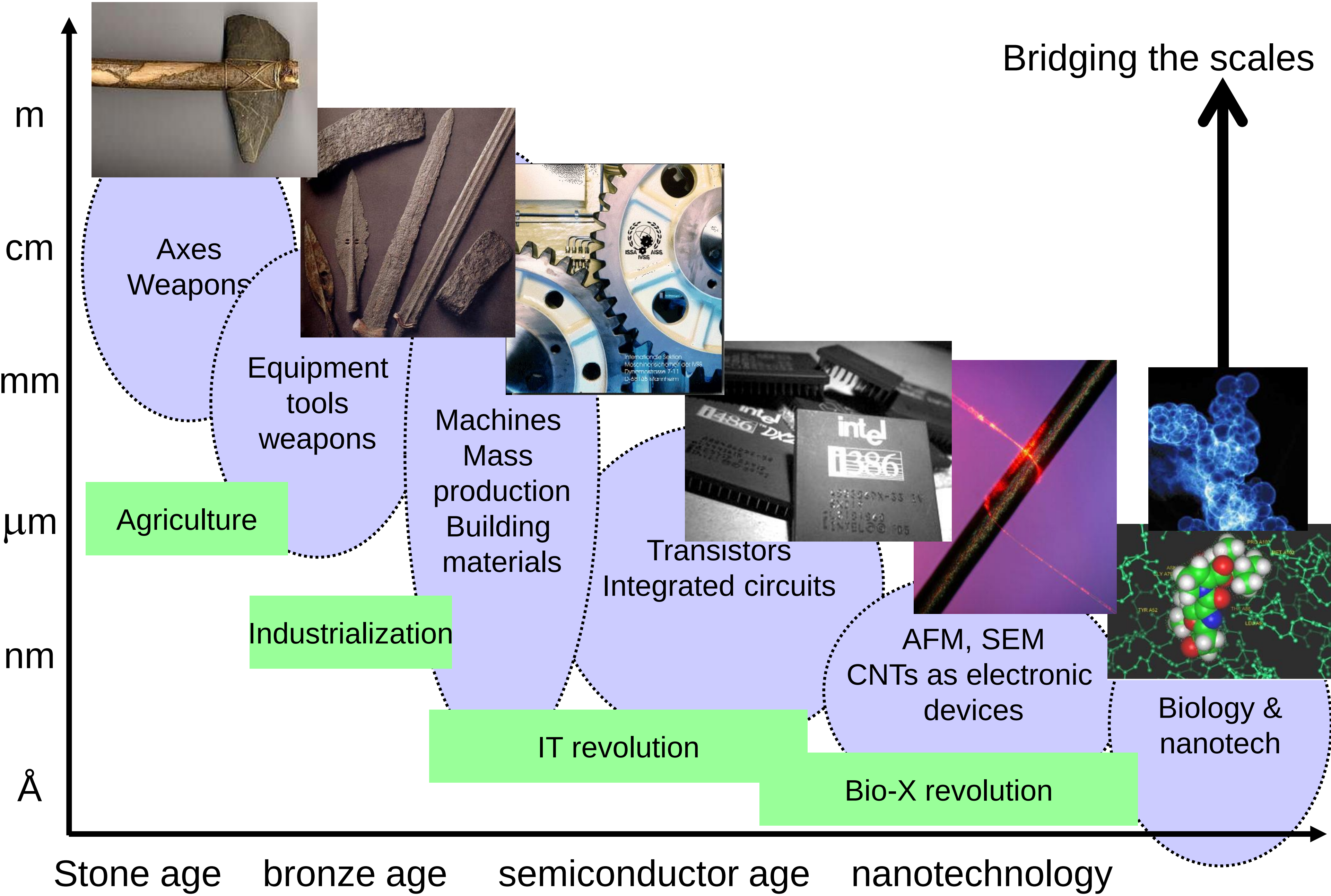
- The lectures will provide an **exposure to several areas of application, based on the scientific exploitation of the power of computation,**

Engineering science paradigm: Multi-scale view of materials



Buehler and Ackbarow, *Materials Today*, 2007

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



Content overview

I. Fundamentals of particle methods

Lectures 1-13
February/March

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

II. Quantum mechanical methods

Lectures 14-24
April/May

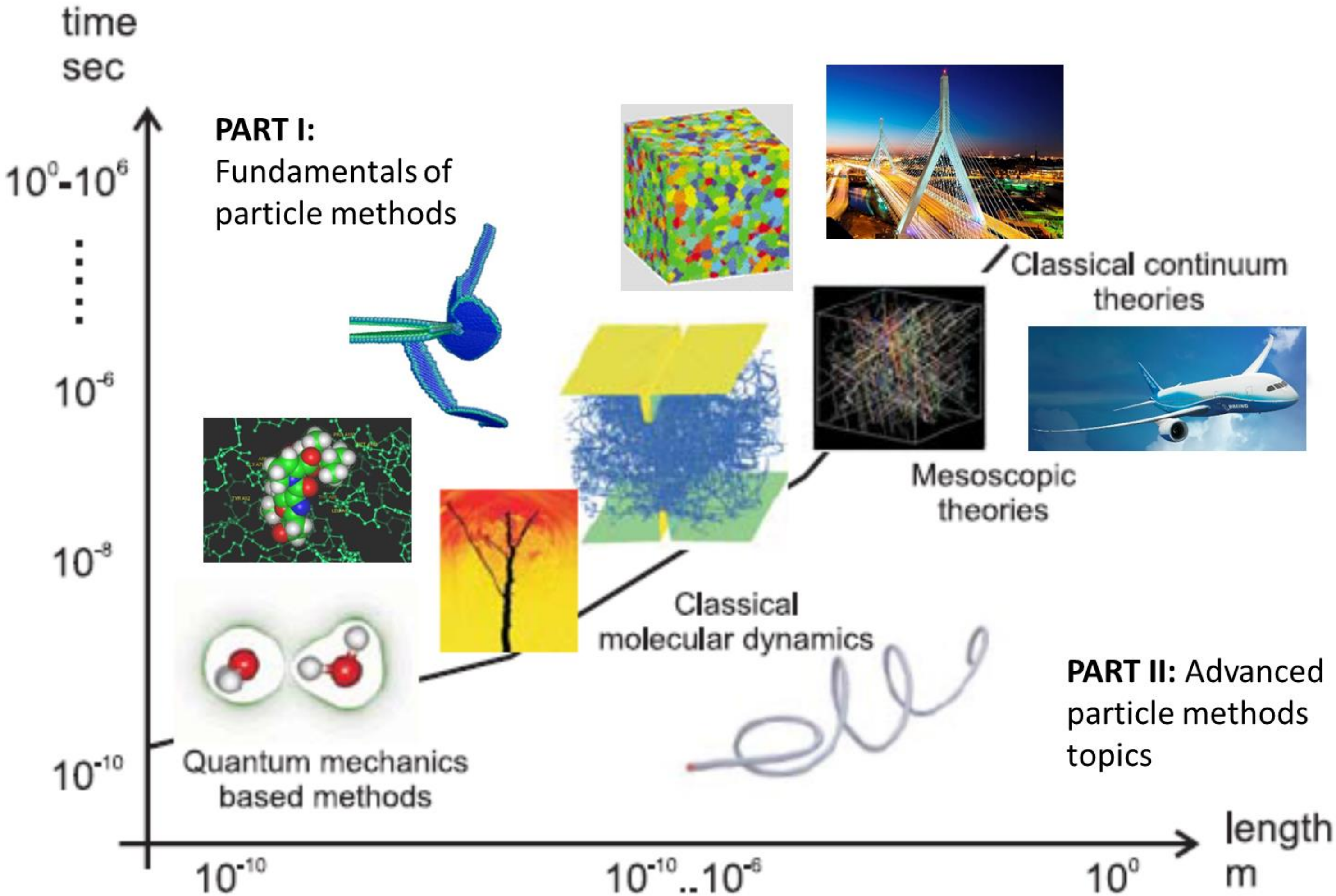
1. Particle? Wave? The principles of quantum mechanics
2. Simple quantum models with analytical solutions
3. The many body problem and numerical solutions
4. Quantum simulations application: storing and converting electrical energy
5. From atoms to solids
6. Properties of materials
7. Machine learning in modelling of physical systems

Schedule IM/S 2018

- **Lecture 1 (Tuesday 2/6): Introduction**
- Recitation #1 (Thursday 2/8): Getting set up for nanoHUB, VMD visualization, etc.
- Lecture 3 (Tuesday 2/12): Basic Molecular Dynamics
- Lecture 4 (Thursday 2/15): Property calculation I
- Lecture 5 (Thursday 2/22): Property calculation II
- Lecture 6 (Tuesday 2/27): How to model chemical interactions: Force fields
- Lecture 7 (Thursday 3/1): Pair potentials and applications to brittle fracture
- Lecture 8 (Tuesday 3/6): Models for polymers and proteins
- Lecture 9 (Thursday 3/9): Examples and applications
- Lecture 10 (Tuesday 3/13): Embedded Atom Method (EAM) & Reactive Force Fields
- Lecture 11 (Thursday 3/15): Reactive force fields and advanced sampling methods
- Lecture 12 (Tuesday 3/20): Review session
- Quiz I: Thursday March 22

"molecular" (explicitly resolve molecules/atoms)
Molecular Dynamics

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

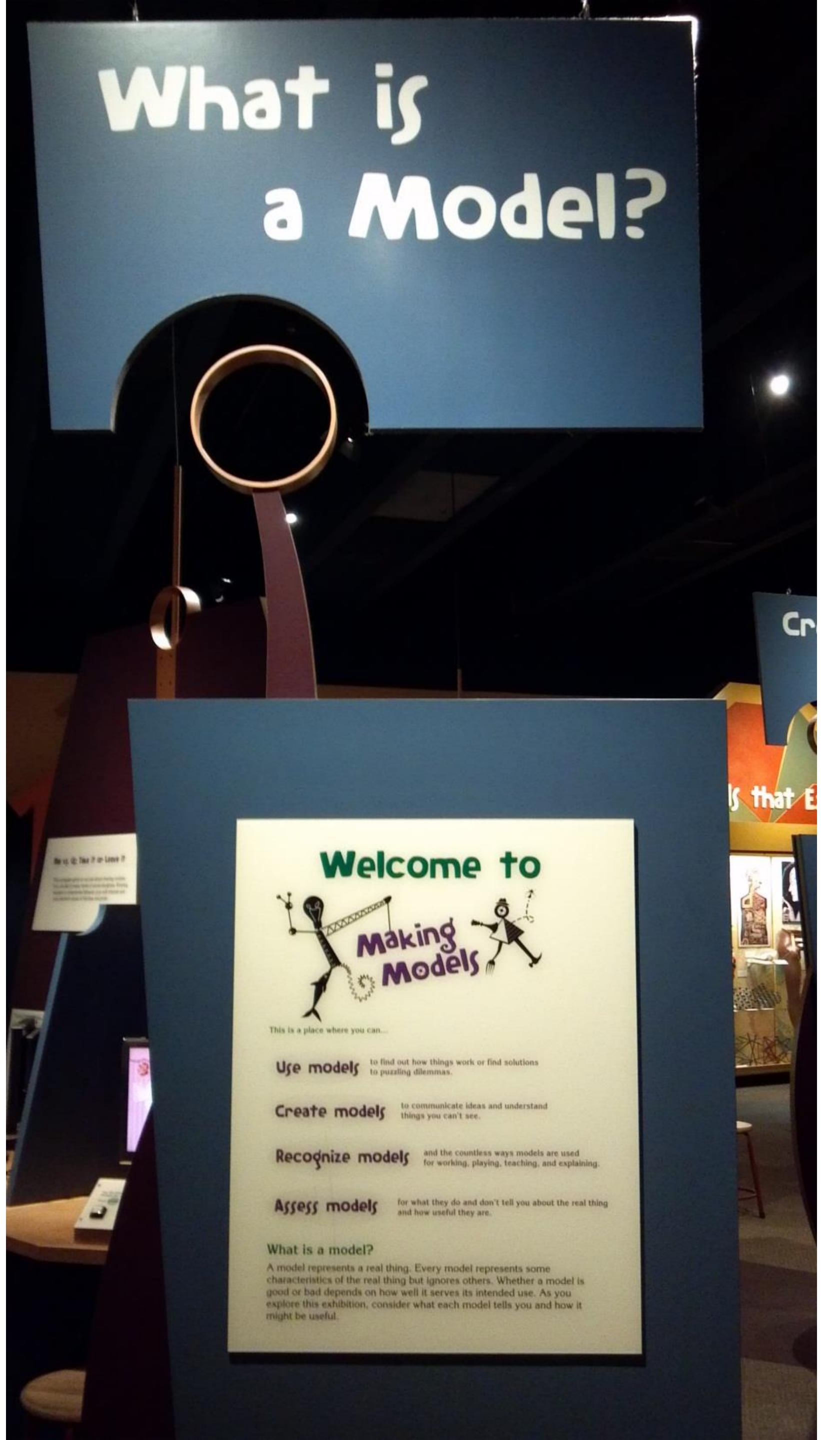


"quantum" (explicitly resolve electrons);
e.g. Density Functional Theory

A few important concepts in modeling and simulation

What is the difference between modeling and simulation?

Museum of Science (Boston)

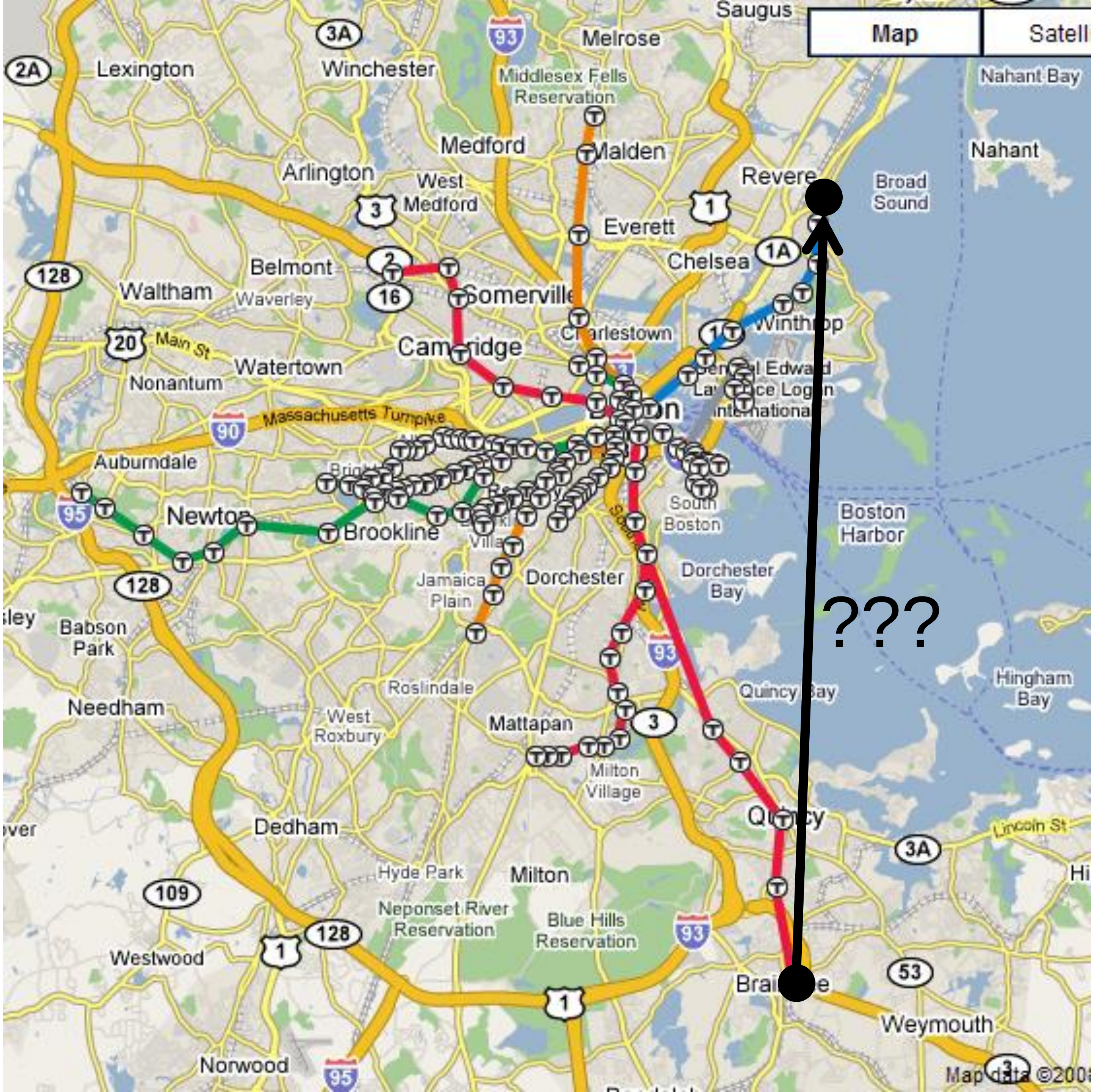



Welcome to
Making Models
This is a place where you can...
Use models to find out how things work or find solutions to puzzling dilemmas.
Create models to communicate ideas and understand things you can't see.
Recognize models and the countless ways models are used for working, playing, teaching, and explaining.
Assess models for what they do and don't tell you about the real thing and how useful they are.
What is a model?
A model represents a real thing. Every model represents some characteristics of the real thing but ignores others. Whether a model is good or bad depends on how well it serves its intended use. As you explore this exhibition, consider what each model tells you and how it might be useful.

Modeling and simulation

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

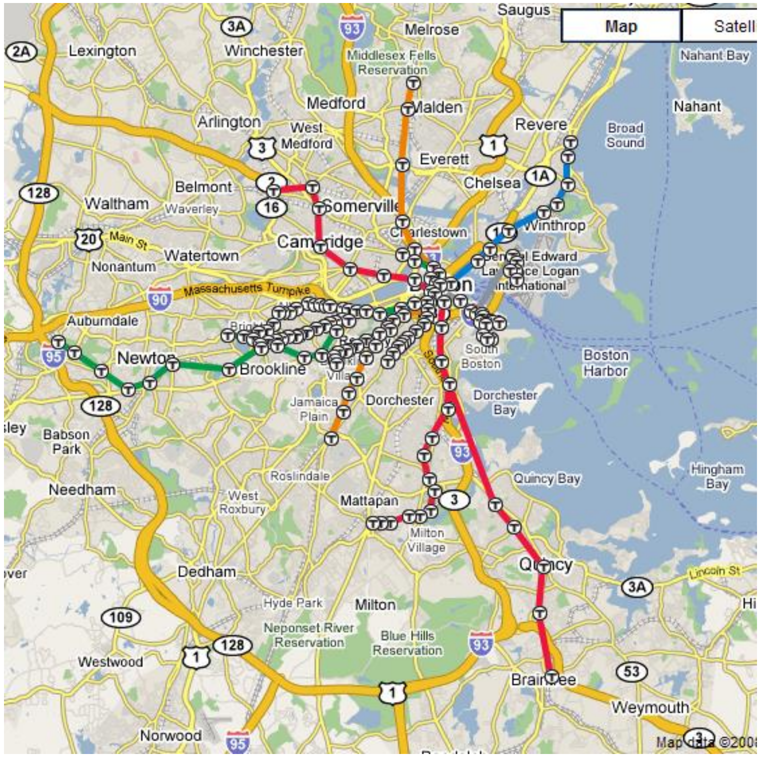
- On the other hand, *simulation* refers to the procedure of solving the equations that resulted from model development.


Map
Satell
???
Saugus
Melrose
Lexington
Winchester
Middlesex Fells Reservation
Nahant Bay
Nahant
Medford
Malden
Arlington
West Medford
Revere
Broad Sound
Everett
Belmont
Chelsea
Waltham
Waverley
Somerville
Winthrop
Cambridge
Charlestown
Watertown
Nonantum
Massachusetts Turnpike
Auburndale
Newton
Brookline
South Boston
Boston Harbor
Dorchester
Dorchester Bay
Jamaica Plain
Babson Park
Needham
Roslindale
West Roxbury
Mattapan
Quincy Bay
Hingham Bay
Milton Village
Quincy
Dedham
Hyde Park
Milton
Neponset River Reservation
Blue Hills Reservation
Westwood
Weymouth
Norwood
Lincoln St
Map data ©2008

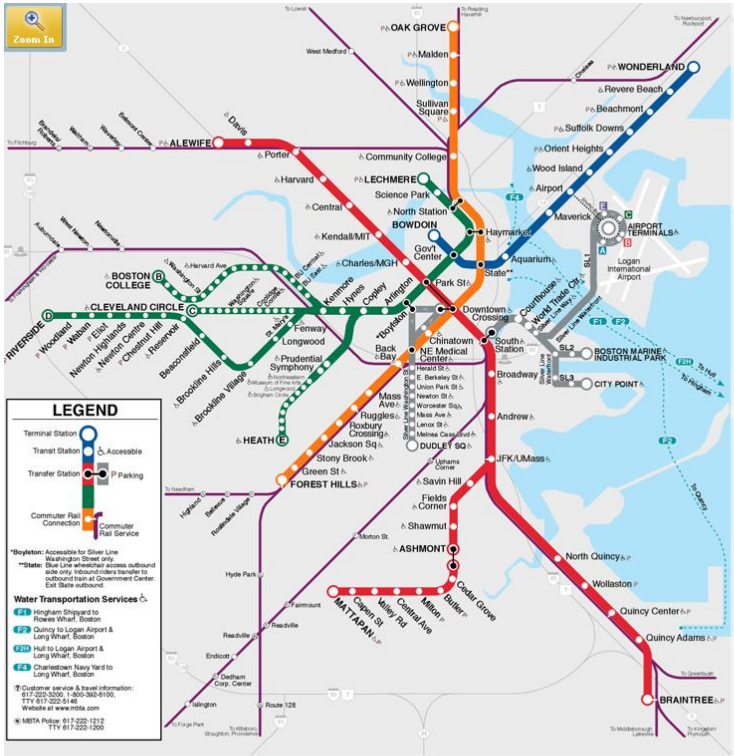
What is a model?

Mike Ashby (Cambridge University):

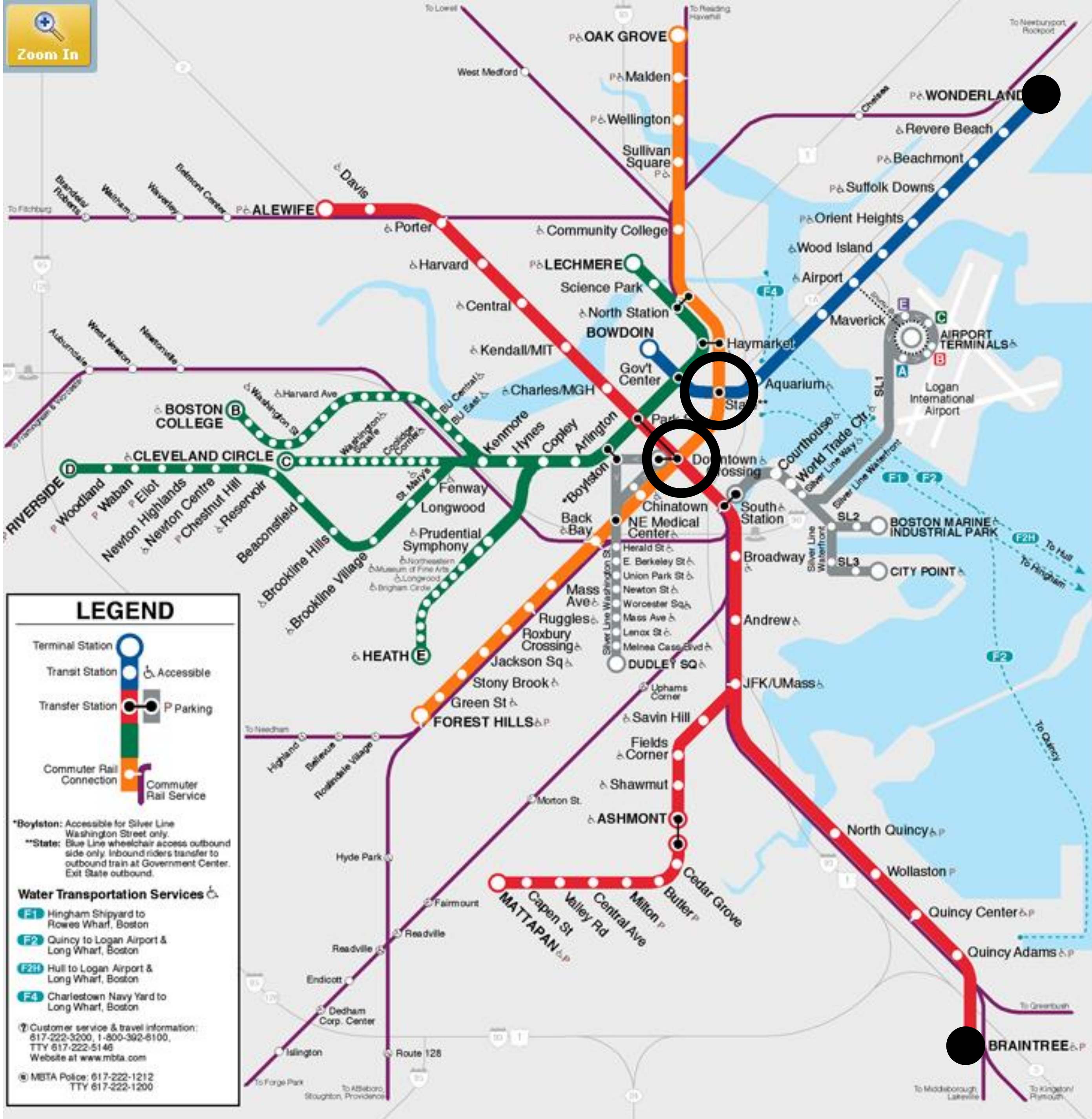
- *A model is an idealization. Its relationship to the real problem is like that of the map of the London tube trains to the real tube systems: a gross simplification, but one that captures certain essentials.*



"Physical situation"



"Model"


Zoom In
OAK GROVE
Malden
Wellington
Sullivan Square
Community College
WONDERLAND
Revere Beach
Beachmont
Suffolk Downs
Orient Heights
Wood Island
Airport
Maverick
AIRPORT TERMINALS
Logan International Airport
Chelsea
ALEWIFE
Davis
Porter
Harvard
Central
Kendall/MIT
Charles/MGH
LECHMERE
Science Park
North Station
BOWDOIN
Haymarket
Gov't Center
Aquarium
State**
Park St
Downtown Crossing
Courthouse
World Trade Ctr.
South Station
Chinatown
NE Medical Center
Broadway
Andrew
JFK/UMass
Savin Hill
Fields Corner
Shawmut
ASHMONT
Cedar Grove
Butler
Milton
Central Ave
Valley Rd
Capen St
MATTAPAN
North Quincy
Wollaston
Quincy Center
Quincy Adams
BRAINTREE
BOSTON COLLEGE
CLEVELAND CIRCLE
RIVERSIDE
Woodland
Waban
Eliot
Newton Highlands
Newton Centre
Chestnut Hill
Reservoir
Beaconsfield
Brookline Hills
Brookline Village
Kenmore
Hynes
Copley
Arlington
*Boylston
Fenway
Longwood
Prudential
Symphony
HEATH
Back Bay
Mass Ave
Ruggles
Roxbury Crossing
Jackson Sq
Stony Brook
Green St
FOREST HILLS
BOSTON MARINE INDUSTRIAL PARK
CITY POINT
Herald St
E. Berkeley St
Union Park St
Newton St
Worcester Sq
Mass Ave
Lenox St
Melnea Cass Blvd
DUDLEY SQ
LEGEND
Terminal Station
Transit Station
Accessible
Transfer Station
P Parking
Commuter Rail Connection
Commuter Rail Service
*Boylston: Accessible for Silver Line Washington Street only.
**State: Blue Line wheelchair access outbound side only. Inbound riders transfer to outbound train at Government Center. Exit State outbound.
Water Transportation Services
F1 Hingham Shipyard to Rowes Wharf, Boston
F2 Quincy to Logan Airport & Long Wharf, Boston
F2H Hull to Logan Airport & Long Wharf, Boston
F4 Charlestown Navy Yard to Long Wharf, Boston
Customer service & travel information: 617-222-3200, 1-800-392-6100, TTY 617-222-5146
Website at www.mbta.com
MBTA Police: 617-222-1212 TTY 617-222-1200

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.*

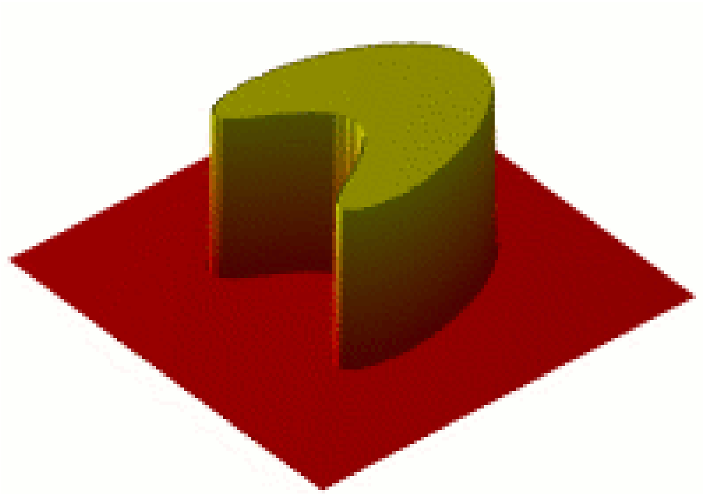
- *At worst, a model is a concise description of a body of data. At best, it captures the essential physics of the problem, it illuminates the principles that underline the key observations, and it predicts behavior under conditions which have not yet been studied.*

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



Oleg Alexandrov

Survey and feedback

Lecture 3 - questions

1. Explain the basic concept of molecular dynamics.
2. Can you see a difference in the Mean Square Displacement function that allows you to distinguish a crystal solid, liquid, gas? Explain details.
3. Explain the concept of “ensemble”. Describe using the terms microscopic and macroscopic states.
4. Explain using a simple schematic why one can not use a single microscopic state to calculate macroscopic properties, e.g. use the temperature as property.
5. Write an expression how to calculate the macroscopic ensemble average of a quantity A from microscopic states.
6. Explain in 2-3 sentences how to use the Monte Carlo approach to calculate the value of π.
7. The MC approach generates a series of microscopic states. To calculate the macroscopic ensemble average, do you need to weight the properties of individual microscopic states?.

8. Were the goals of today’s lecture clear?
9. Was today’s lecture clear?
10. Did you feel that today’s lecture contributed to your understanding of the topic?
11. What could have been improved in order to make this lecture more useful?
12. Is the level of teaching appropriate? What should we change?

13. Please give us overall feedback regarding IM/S so far (overall usefulness, how interesting are lectures, overall impression, suggestions for changes, etc.).

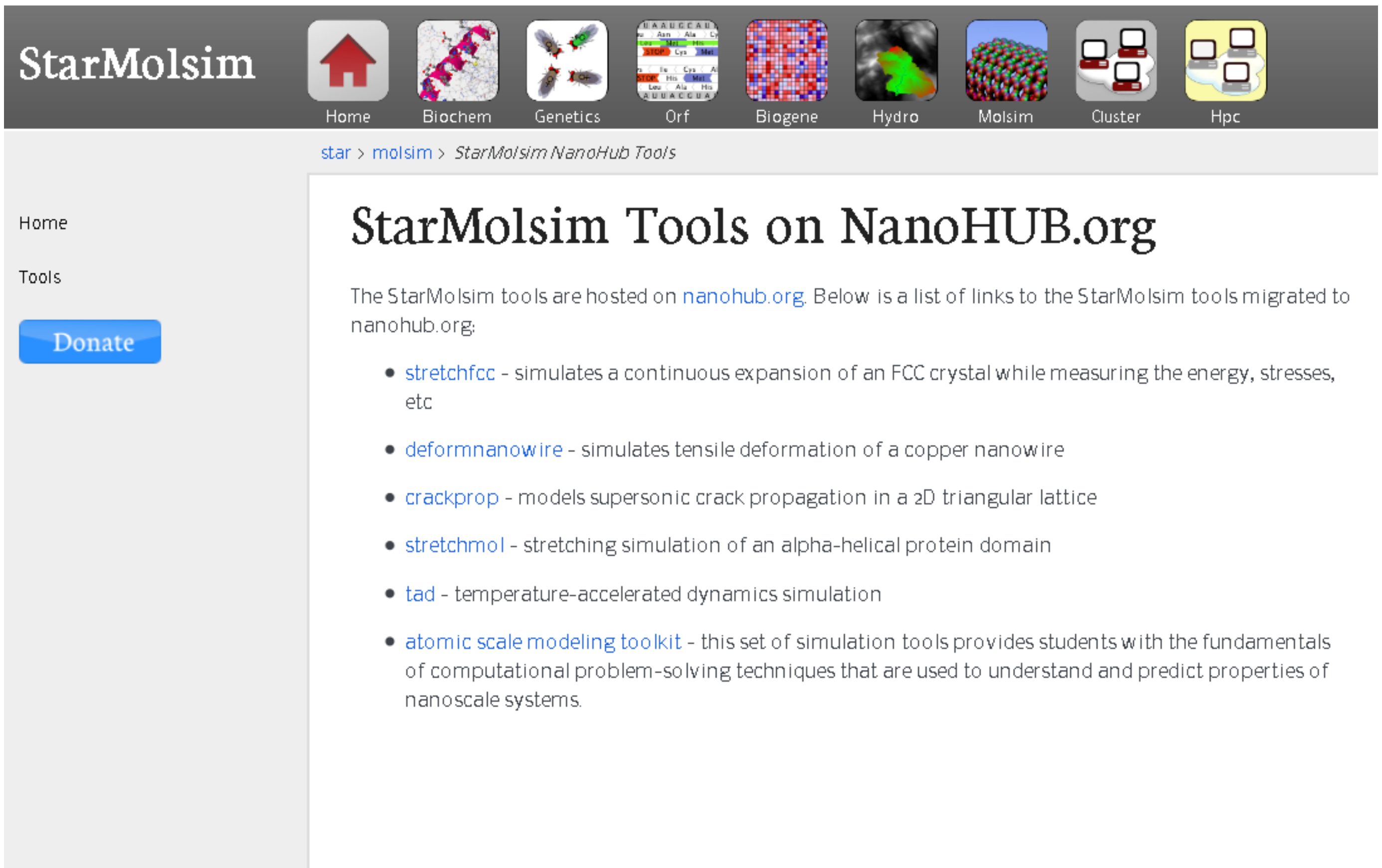
For most applications, we will use a website-driven simulation framework developed in collaboration with MIT's Office for Undergraduate Education

nanoHUB: *https://nanohub.org*

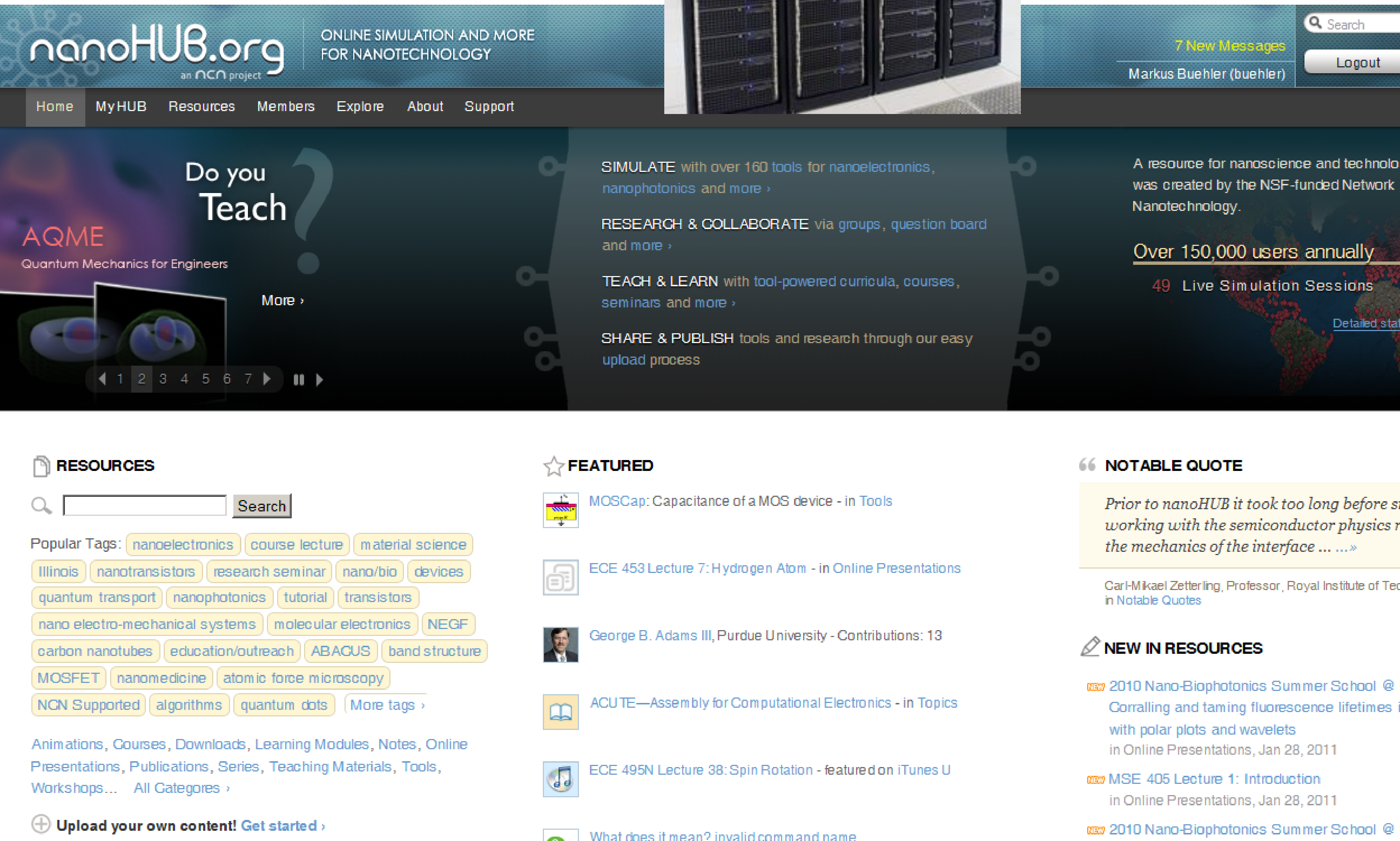
More than 200 tools:
https://nanohub.org/resources/tools

Our own IM/S nanoHUB tools

URL:
http://web.mit.edu/star/molsim/nanohub/index.html



Real cluster runs in the back



Nanowire Tensile Deformation Lab

1 Input → 2 Run Experiment

About this tool
Questions?

Crystal Structure | Limits | Boundary Conditions | Simulation Parameters

Dimension_x (even integer): 4

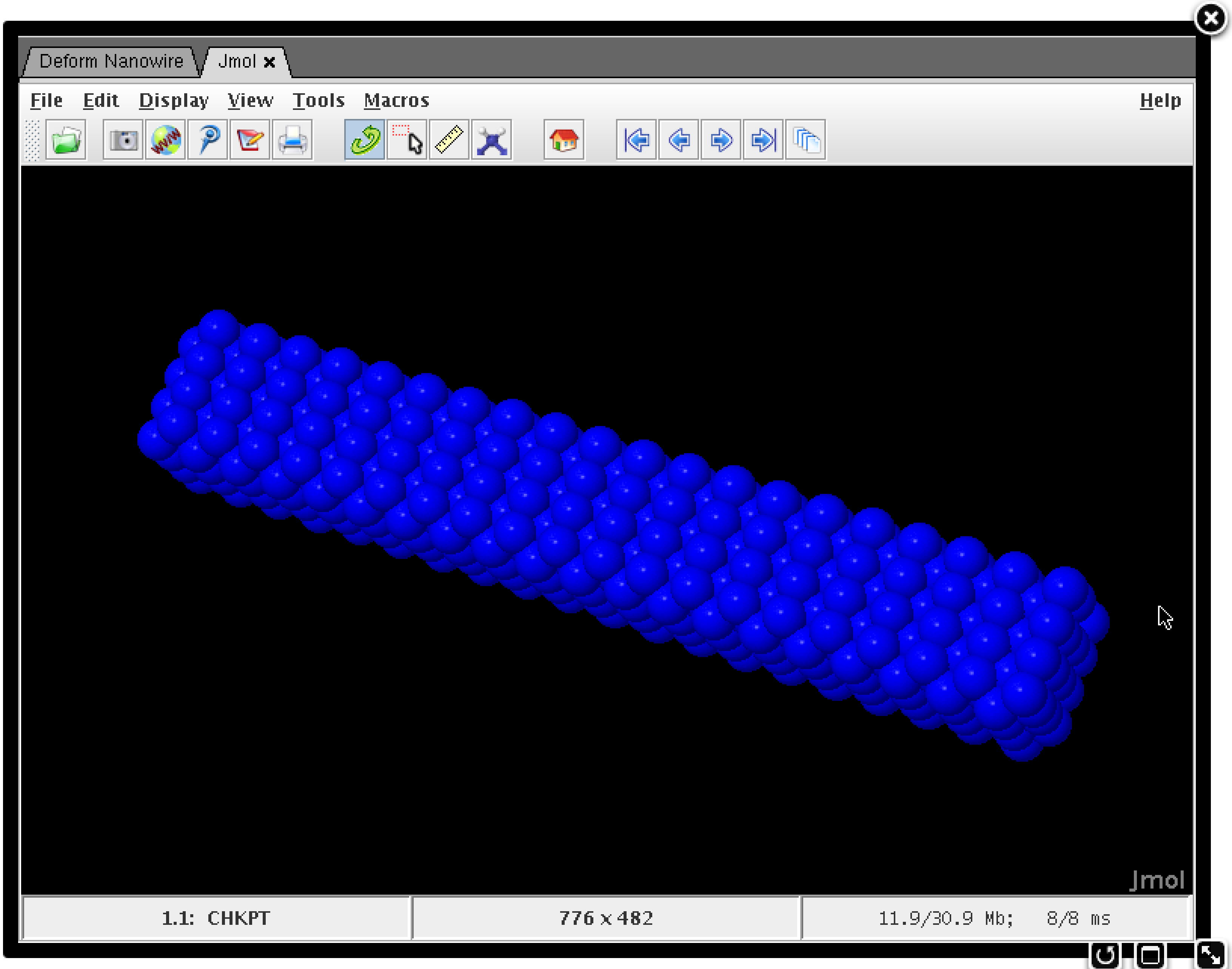
Dimension_y (even integer): 4

Dimension_z (even integer): 4

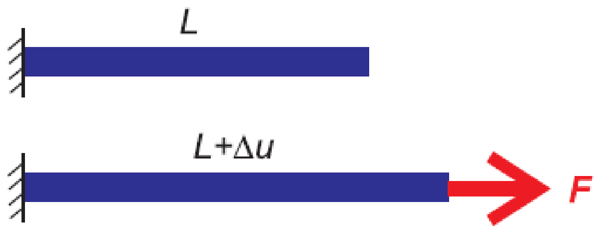
Software Tools for Academics and Researchers
Office of Educational Innovation and Technology

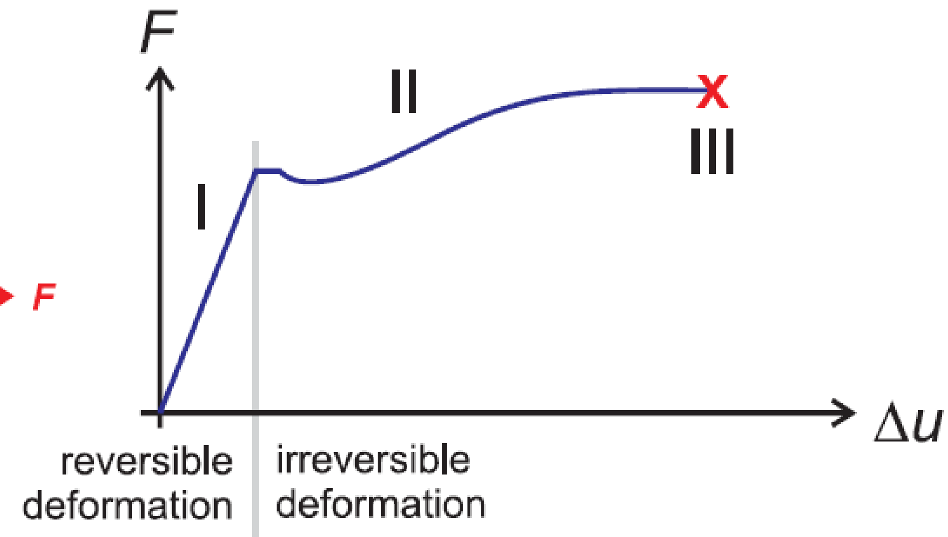
Massachusetts Institute of Technology

Run Experiment >

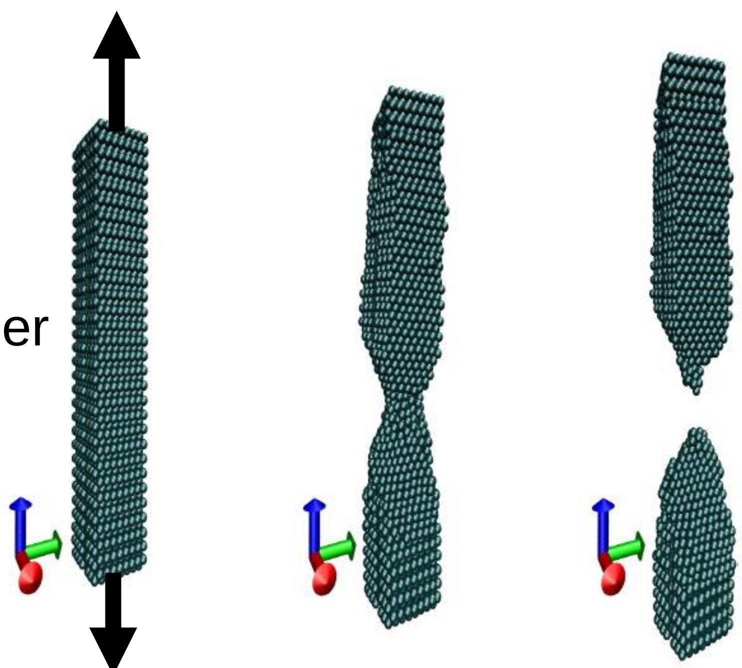

Deform Nanowire
Jmol
File
Edit
Display
View
Tools
Macros
Help
Jmol
1.1: CHKPT
776 x 482
11.9/30.9 Mb; 8/8 ms

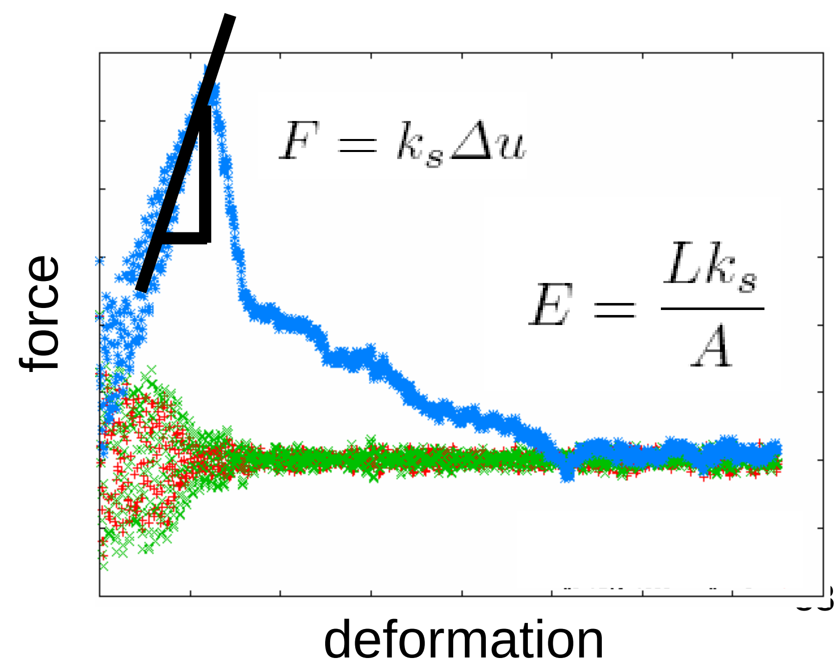
Example: Stretching nanowire





copper





Content overview

I. Fundamentals of particle methods

Lectures 1-13
February/March

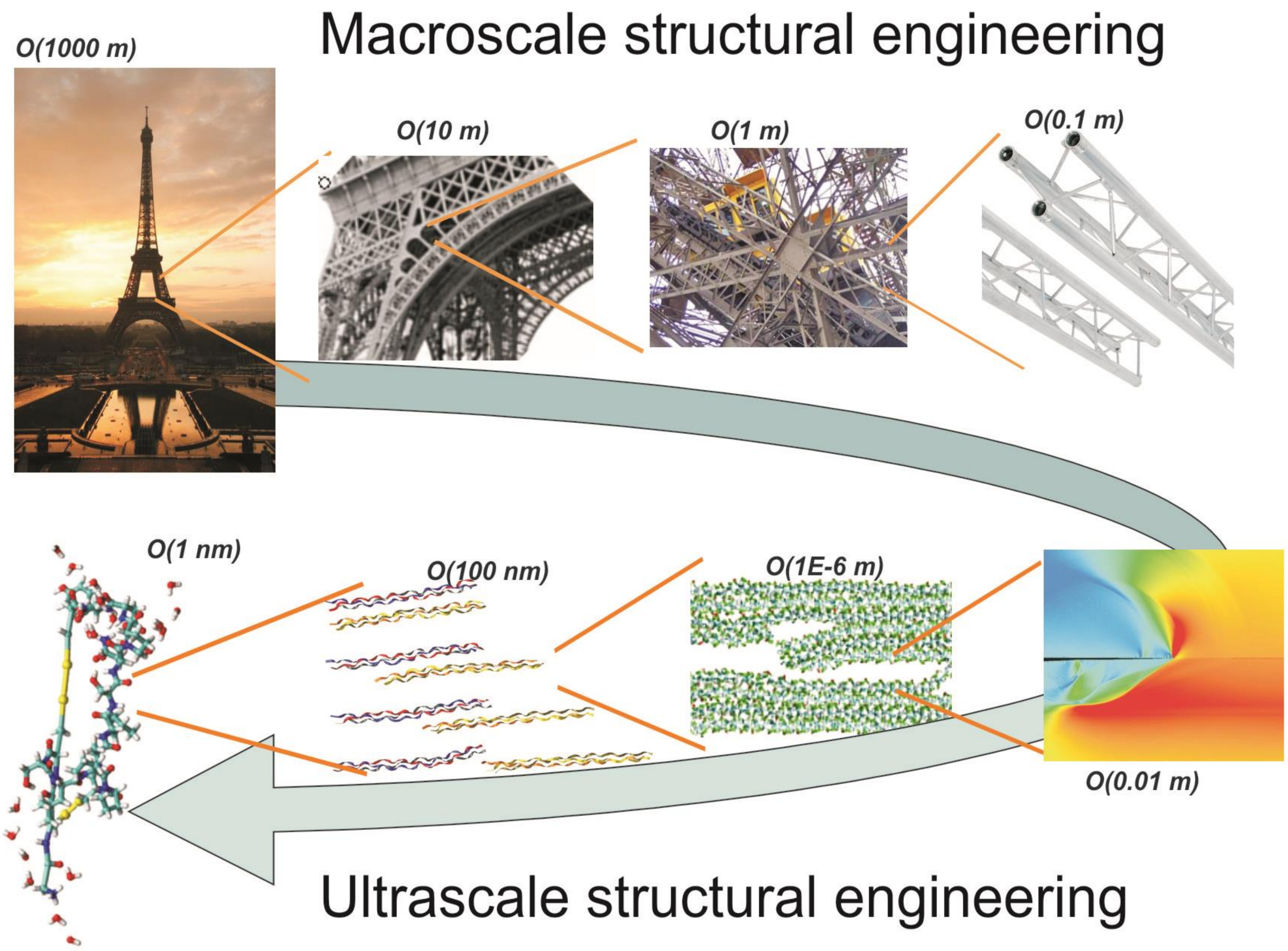
1. Atoms, molecules, chemistry
2. Statistical mechanics
3. Molecular dynamics, Monte Carlo
4. Visualization and data analysis
5. Mechanical properties – application: how things fail (and how to prevent it)
6. Multi-scale modeling paradigm
7. Biological systems (simulation in biophysics) – how proteins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

II. Quantum mechanical methods

Lectures 14-24
April/May

1. Particle? Wave? The principles of quantum mechanics
2. Simple quantum models with analytical solutions
3. The many body problem and numerical solutions
4. Quantum simulations application: storing energy
5. From atoms to solids
6. Properties of materials
7. Machine learning in modelling of physical systems

Multi-scale view of materials

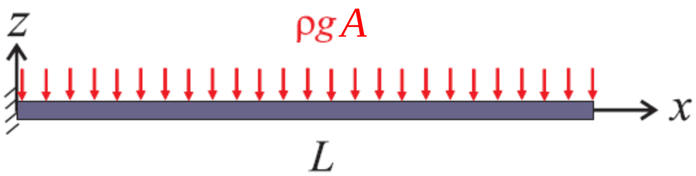


Buehler and Ackbarow, *Materials Today*, 2007

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

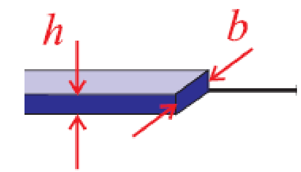
Governing equation (PDE)

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

Integration & BCs

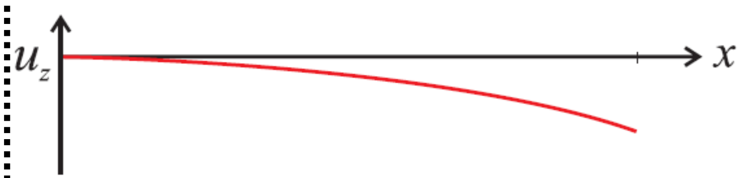
Geometry

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



BC - load:

$$\rho g A$$



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

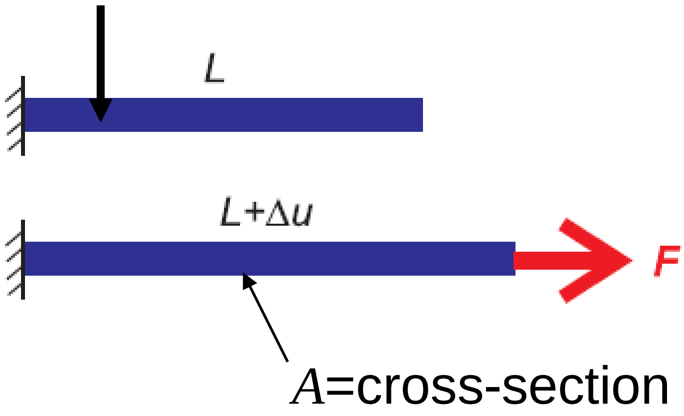
E = unknown parameter

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)

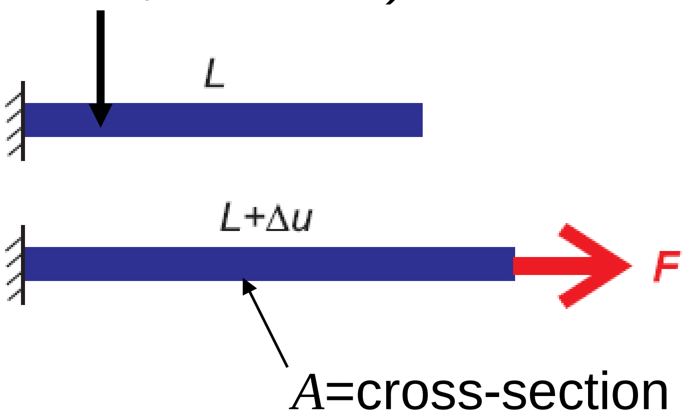


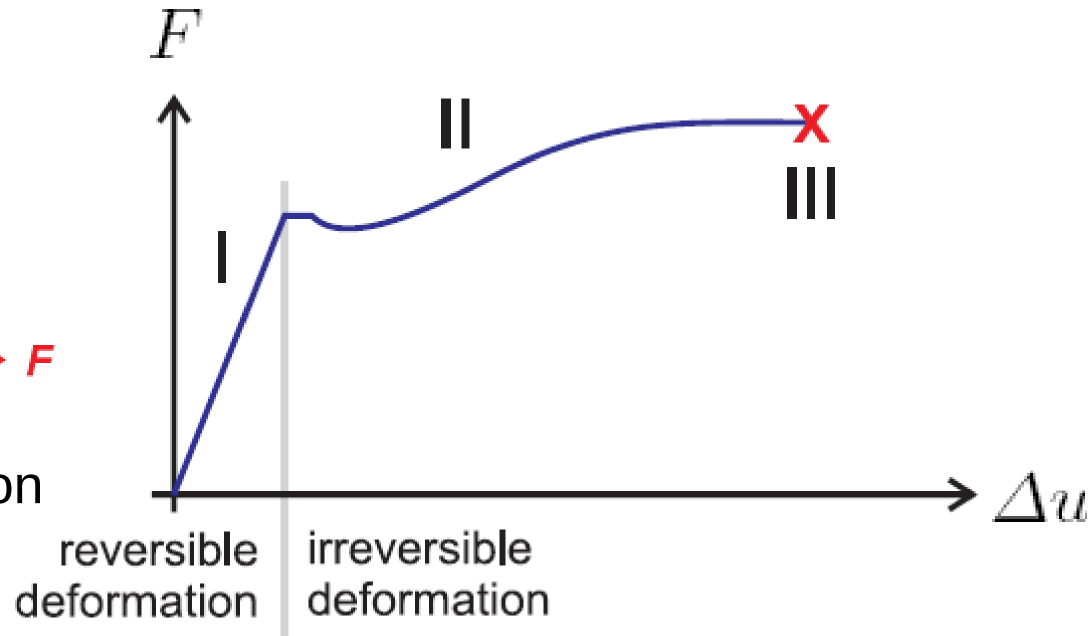
http://img.directindustry.com/images_di/photo-g/tensile-compression-testing-machine-41713.jpg

How to determine Young's modulus E ?

Measurement (laboratory):

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

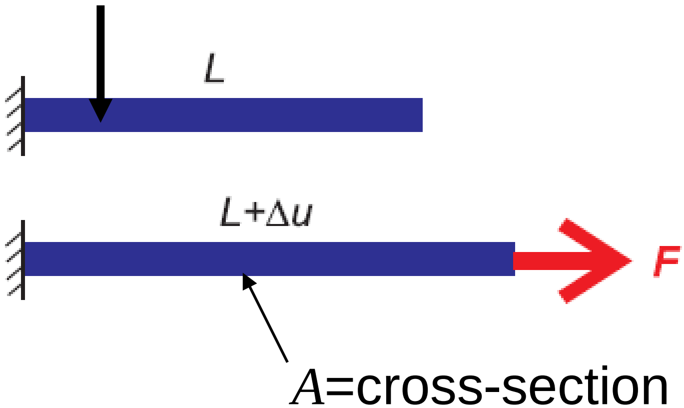


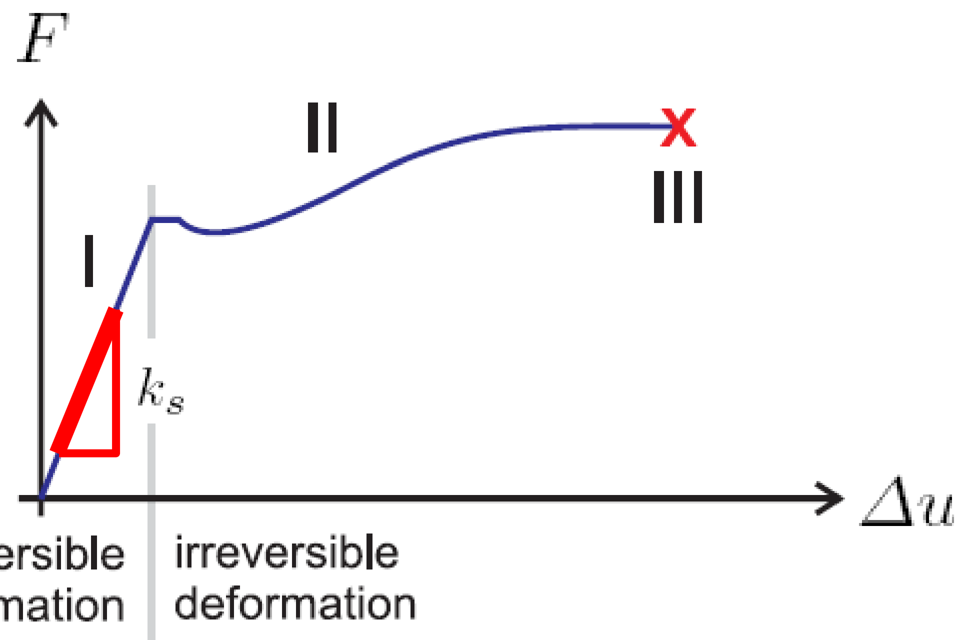


How to determine Young's modulus E ?

Measurement (laboratory):

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





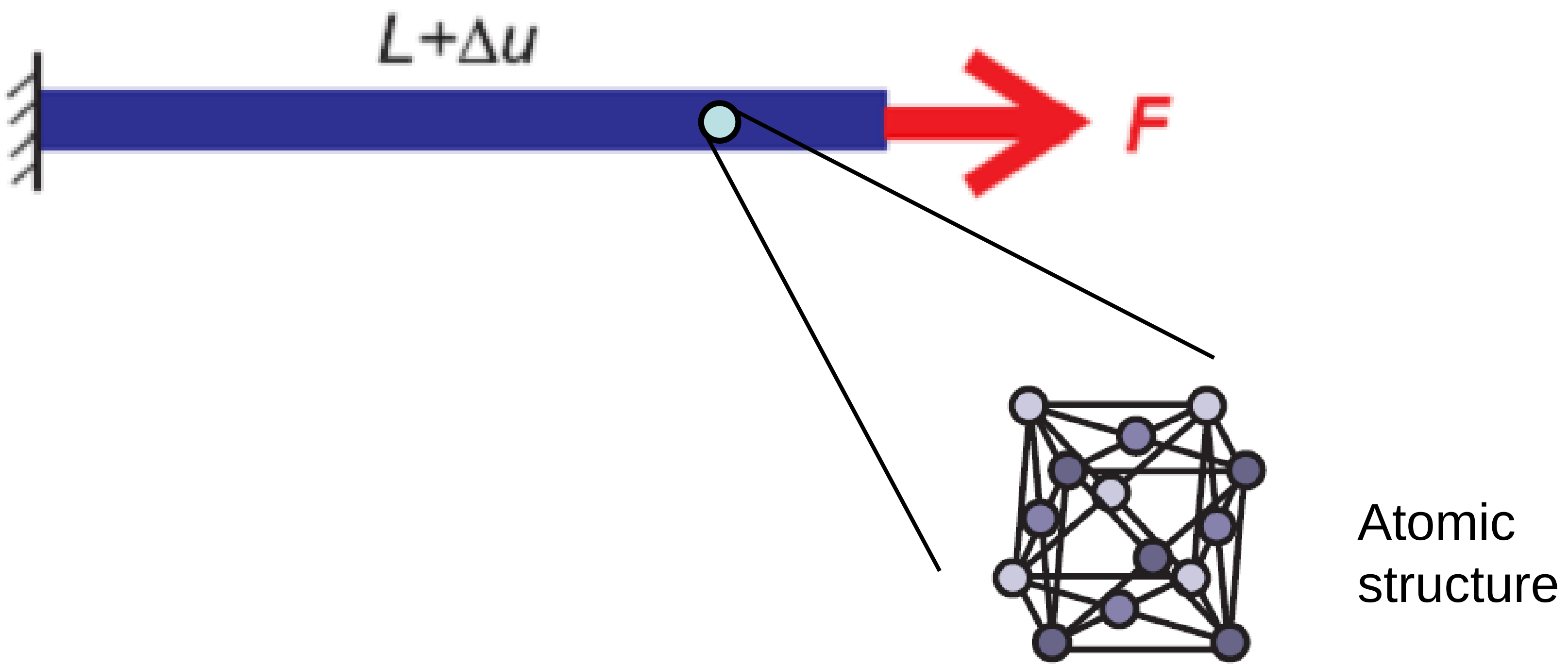
$$F = k_s \Delta u$$

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

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

How to determine E ? - alternative approach to laboratory experiment

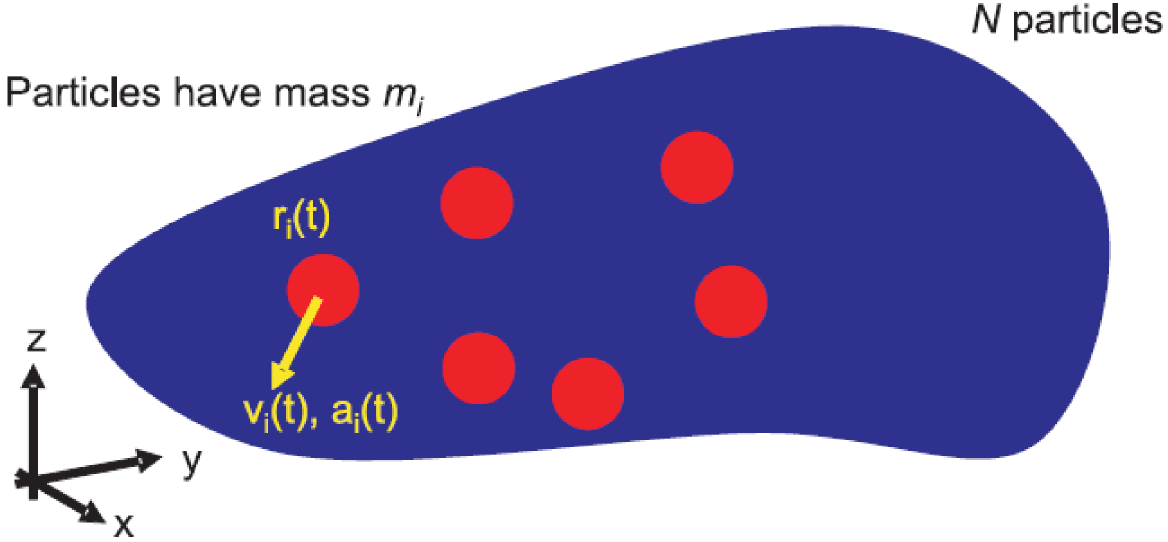
Atomistic simulation – *new engineering paradigm*



Concept: 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…)

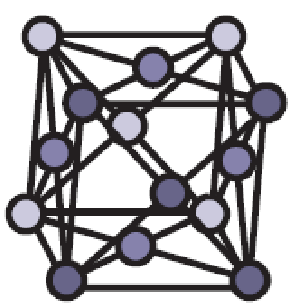


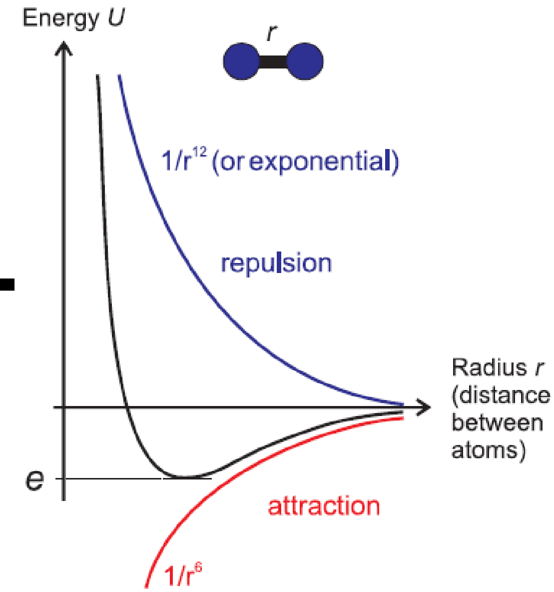
Linking atomistic and continuum perspective

- 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

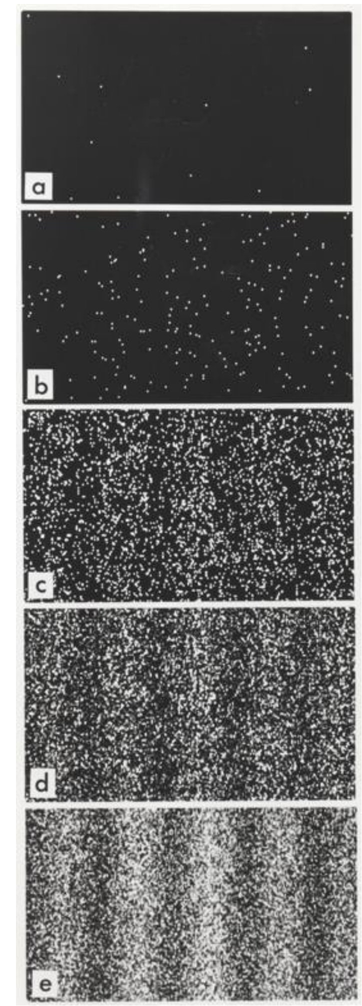
- *Atomistic models provide fundamental perspective, and thereby a means to determine (solely from the atomistic / chemical structure of the material) important parameters to be used in continuum models*





Quantum environment

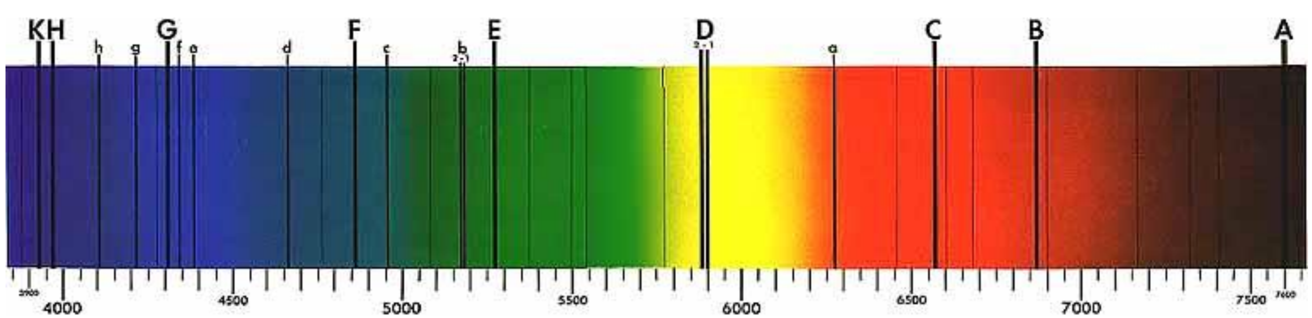
- Quantum mechanics deals with the behavior of matter at very small scales.
- Newtonian physics works well (even at the microscopic scale), but when considering the structure of atoms new phenomena appear without a macroscopic counterpart.



- Wave-particle duality
- Non-determinism
- Indeterminacy
- Superposition
- Entanglement
- Observer effect

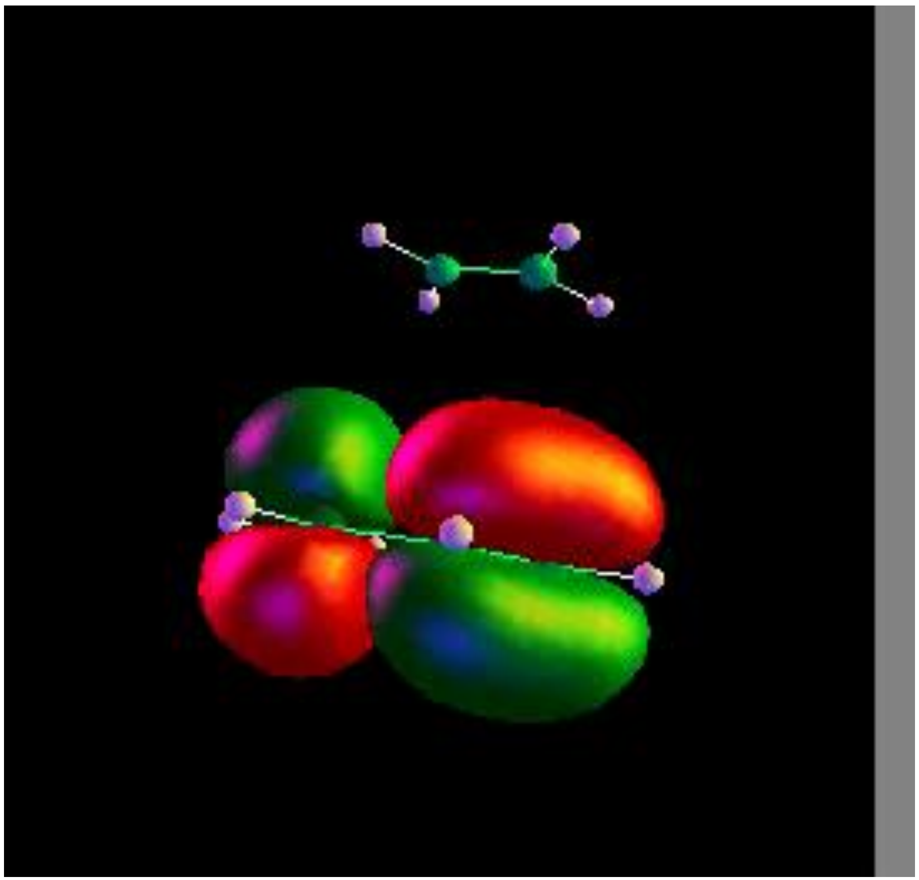
Schrödinger equation

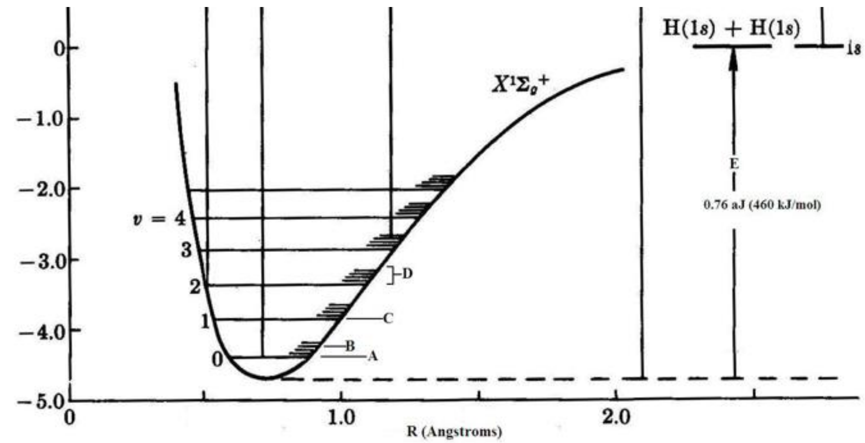
$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}\right)+V\left(x\right)\right]\Psi\left(x\right)=E\Psi\left(x\right)$$

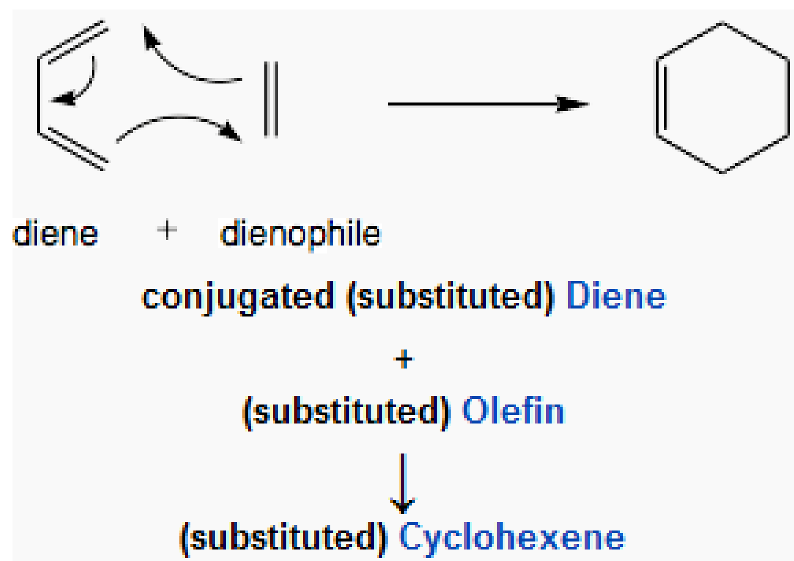


Quantum mechanics

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

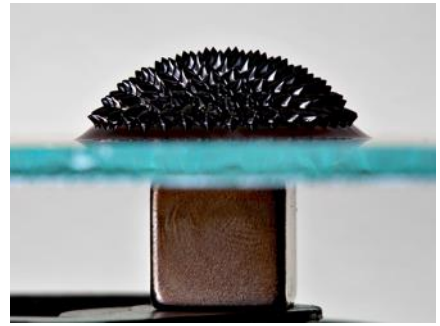
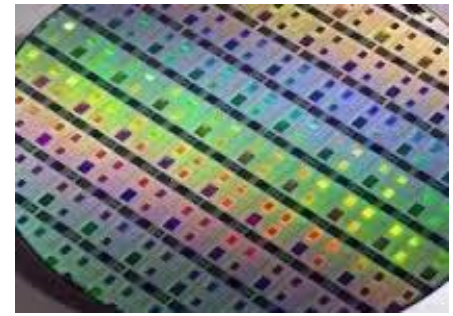




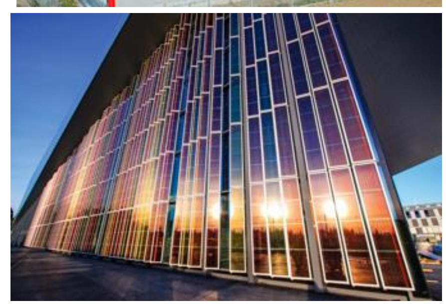


Quantum Materials

Semiconductors
Photovoltaics
Electroluminescence
Photosynthesis
Energy storage and electrochemistry
Photochromes and solar fuels
Nanomaterials



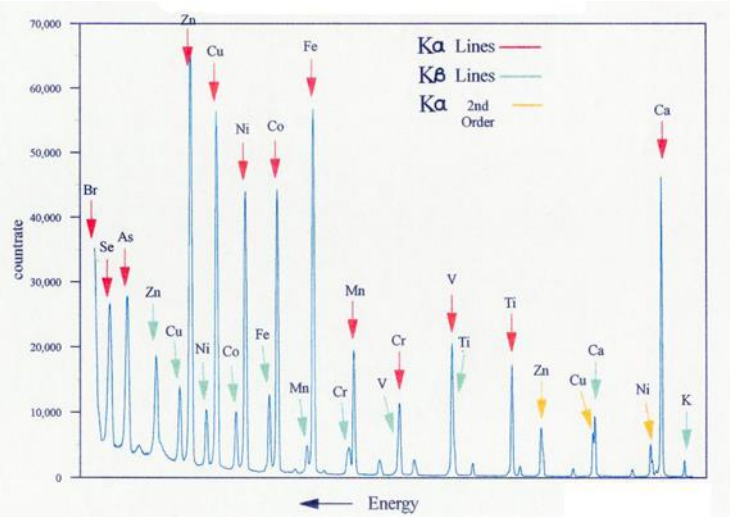


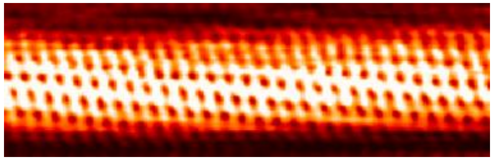

Electrical, optical, magnetic properties …

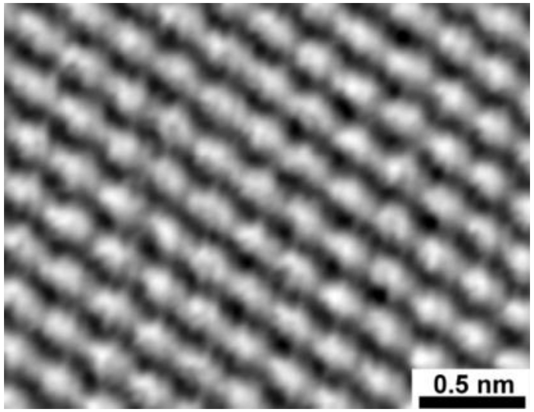
Quantum techniques

Many materials characterization techniques are based on quantum phenomena:

- X-ray photoelectron spectroscopy, Auger electron spectroscopy
- Visible / UV / X-ray fluorescence and photoemission spectroscopy
- Raman and Infrared spectroscopy
- Scanning probe microscopy (Scanning tunneling microscope, Atomic force microscopy, …)







Quantum Modeling and Simulation

- We can solve the Schrödinger equation with as much accuracy as we want … but we need a computer larger than the universe.
- Need to develop models that are as simple as possible and still capture the quantum effects. Depending on method, we can address 10s – 1000s atoms
- Use accurate simulations to supply parameters for simpler models.

- Use simulation to go after the **Inverse Design** problem:
  Given target performance, which is the optimal material?

In Section two, you will

- build simple quantum models
- understand the key quantum effects that they need to capture
- run simulations using these models and extract conclusions from them
- analyze how M&S accelerates discovery of materials
- test how machine learning can assist in M&S

Schedule IM/S 2018

- Lecture 1 (Tuesday 2/6): Introduction
- **Recitation #1 (Thursday 2/8): Getting set up for nanoHUB, VMD visualization, etc.**
- Lecture 3 (Tuesday 2/12): Basic Molecular Dynamics
- Lecture 4 (Thursday 2/15): Property calculation I
- Lecture 5 (Thursday 2/22): Property calculation II
- Lecture 6 (Tuesday 2/27): How to model chemical interactions: Force fields
- Lecture 7 (Thursday 3/1): Pair potentials and applications to brittle fracture
- Lecture 8 (Tuesday 3/6): Models for polymers and proteins
- Lecture 9 (Thursday 3/9): Examples and applications
- Lecture 10 (Tuesday 3/13): Embedded Atom Method (EAM) & Reactive Force Fields
- Lecture 11 (Thursday 3/15): Reactive force fields and advanced sampling methods
- Lecture 12 (Tuesday 3/20): Review session
- Quiz I: Thursday March 22