IOWA STATE UNIVERSITY

Aerospace Engineering Department

Multi Physics/Scale Modeling/Simulation of Nanomaterials

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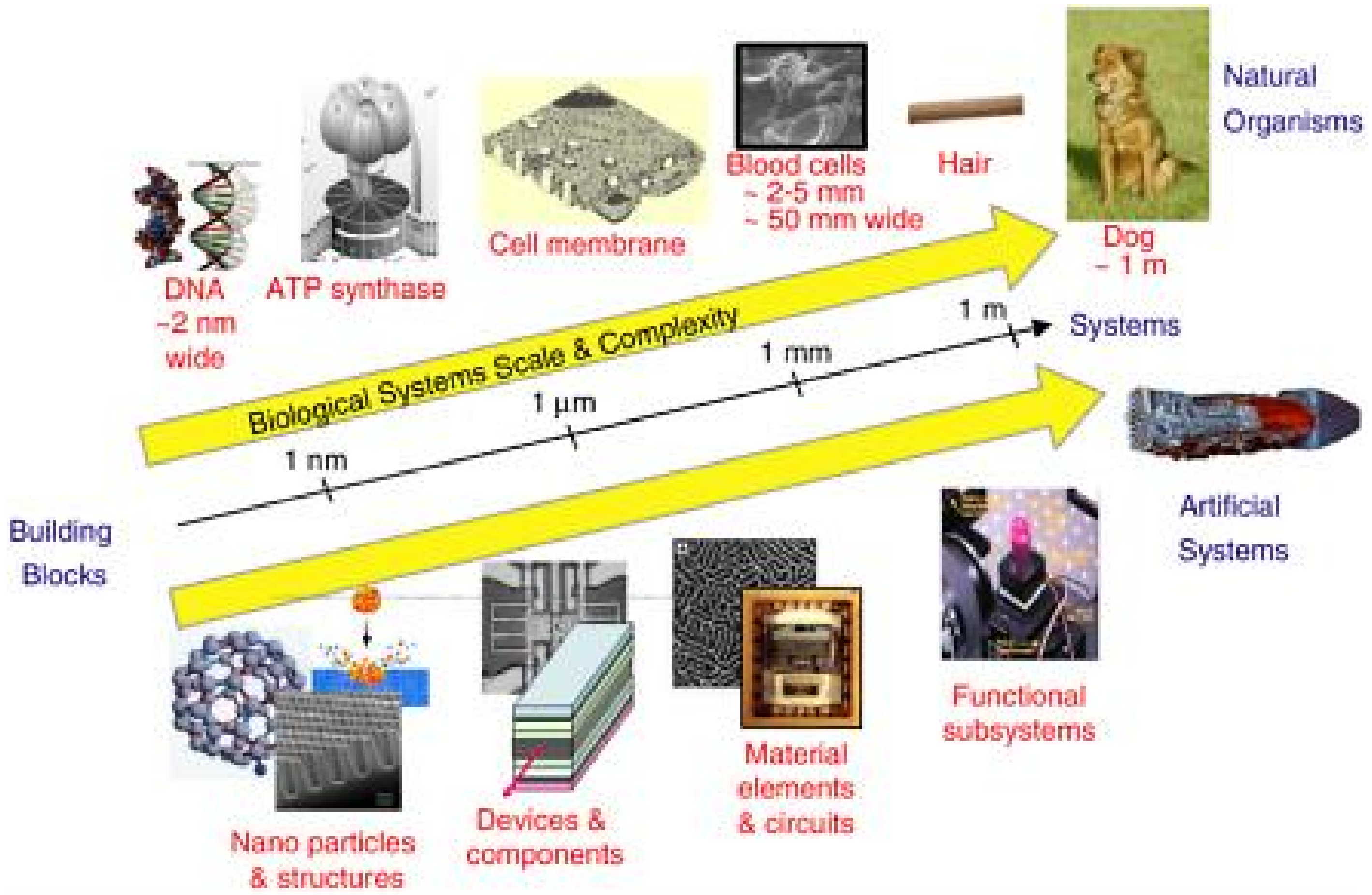
Outline

- Introduction
- Materials Modeling
- Multiphysics
- Multiscale Modeling
- Lab instructions

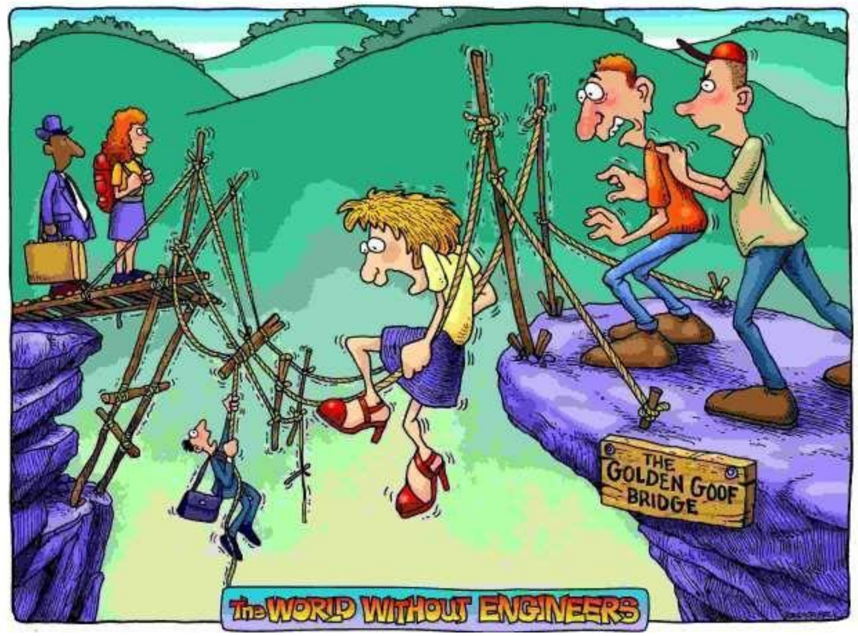
Introduction

- Conceptual view to size…



NOT Mine

Introduction: Significance of Calculations



Introduction: Effect of dimensions

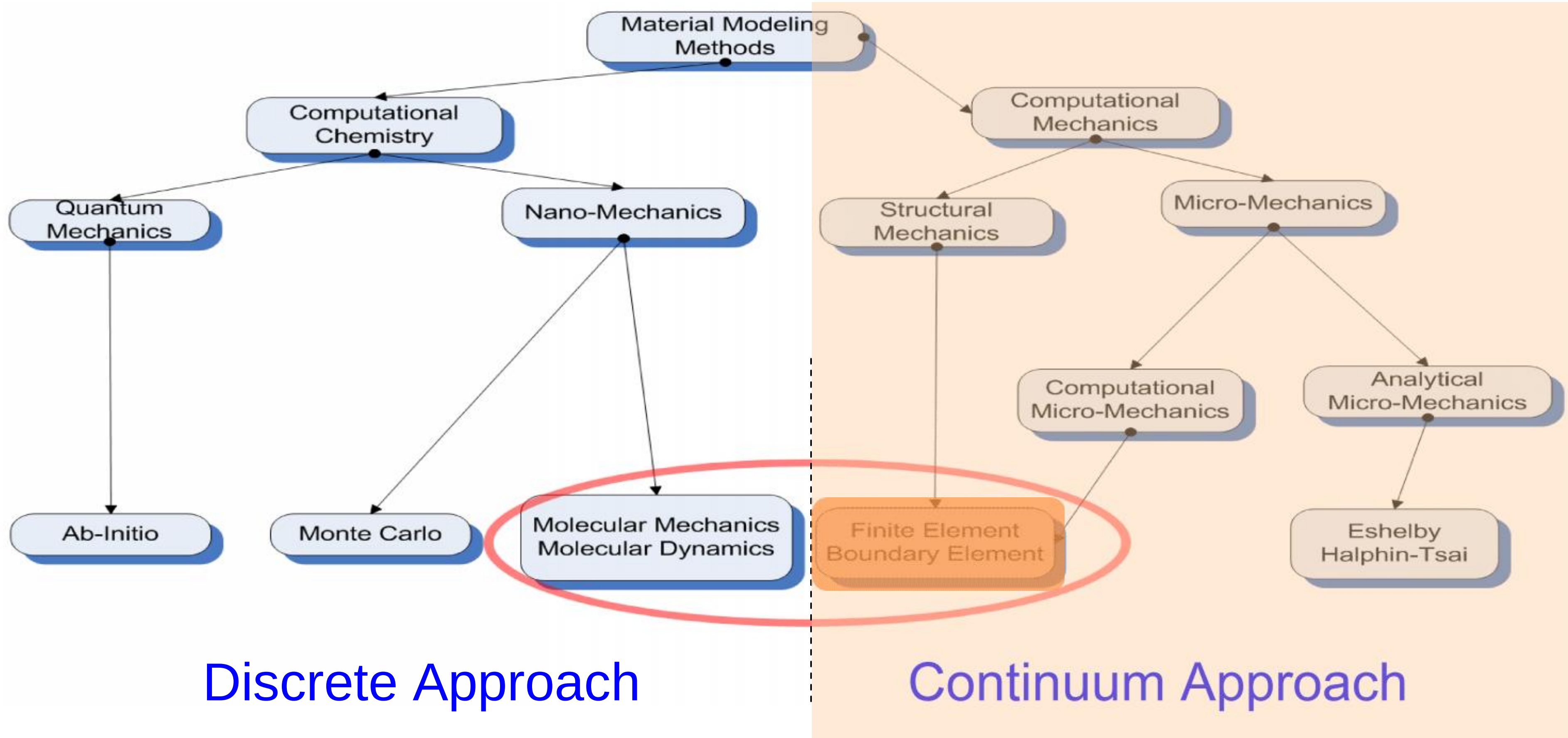
- The mystery of nanoscale

Introduction: Modeling vs. Simulation

- Modeling
  - Simplifying the real system
- Simulation
  - Putting more complexity to the real system
- None of them show real system!!!
- What we do?
  - *Simulating* the *Model*

Molecular Dynamics Simulations, elementary methods J.M. Haile, 1992

Materials Modeling: Techniques



Valavala, P. K., and G. M. Odegard. "Modeling techniques for determination of mechanical properties of polymer nanocomposites." *Rev. Adv. Mater. Sci* 9 (2005): 34-44.

Materials Modeling: Primary Concepts

- Field

  A function that depends on the spatial positions
- Order parameter (Phase-Field variables)

  Continuous variables that define the composition, i.e., state of a material.
- Conserved quantities

  Neither created nor destroyed in a kinetic process, e.g., mass and energy
- Nonconserved quantities

  It can be created or destroyed during a kinetic process

Materials Modeling: Fundamentals

- Thermodynamics

  study of equilibrium states, i.e., time-invariant state variables

- Kinetics

  study of the rates of changes of non-equilibrium systems due to different causes (forces)

Good Model:

A model that captures both thermodynamics and kinetics of a material under influence of external forces correctly and accurately, i.e., closer to what happens in reality.

Balluffi, R. W.; Allen, S. M.; Carter, W. C. Kinetics of Materials; 1st ed. Wiley-Interscience, 2005.

Materials Modeling: Fundamentals (cont.)

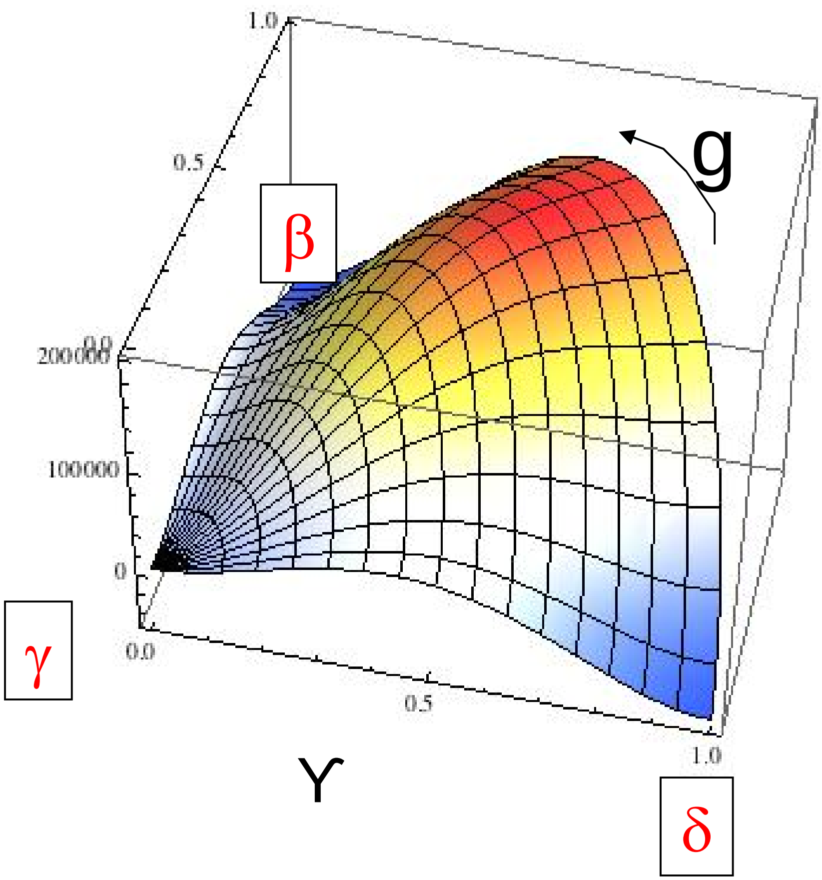
- Basis of kinetic theories:
  - In process with an exchanging extensive property, the equilibrium condition is equality of conjugate potential that is an intensive property
  - A system at equilibrium, with constant potential, has a free energy function that is minimized ➔ A necessary (but not sufficient) condition for equilibrium is ¢ · ≥ 0

▲Modeling of a material is the art of *designing* a *realistic* representative potential function.

Balluffi, R. W.; Allen, S. M.; Carter, W. C. Kinetics of Materials; 1st ed. Wiley-Interscience, 2005.

Materials Modeling: Potential Function

- Requirements
  - Extremum at points corresponding to each metastable phase for any stress and temperature
  - Max value at instability point
  - Captures the energy barriers between phases
  - Do not have artificial minima



Materials Modeling: Irreversible Thermodynamics

- Introduced by Onsager in 1931
- Applies to systems near equilibrium
- Equilibrium ➔ Thermodynamic potential =cte

▲ Nonequilibrium ➔ Thermodynamic potential ≠ cte ≡ spatial variation of potential function

- Thermodynamic functions defined for reversible processes cannot be rigorously used for nonequilibrium processes, ***BUT*** using in close to equilibrium processes ➔ acceptable results

http://en.wikipedia.org/wiki/Lars_Onsager

Materials Modeling: Thermodynamics

Forces

- Near equilibrium ➔ dividing material into cells at equilibrium with local potential function ➔ 1st + 2nd law of thermodynamics

Local form:

$$Tds = du - \sum_j ¤_j d¶_j$$

ϕ : generalized intensive quantity (≡ generalized potential)

ξ : conjugate extensive quantity density (≡ generalized displacement)

Global form:
(Δ local equilibrium)

$$\dot{±} = \mathbf{J}_Q \cdot \nabla \frac{1}{T} - \sum_j \frac{\mathbf{J}_j}{T} \cdot \underbrace{\nabla ¤_j}_{Gen\ Force}$$

Multiphysics

- Linear Irreversible Thermodynamics:
  - Taylor series expansion near equilibrium
  - Ignoring higher order terms

$$J_Q = J_Q(F_Q, F_q, F_1, \ldots, F_{N_c})$$

$$J_\alpha = \sum_\beta L_{\alpha\beta} F_\beta \qquad L_{\alpha\beta} = \frac{\partial J_\alpha}{\partial F_\beta}$$

A multiphysics problem is:

$$L_{\sim}\left(1-\text{¢}_{\sim}\right)\neq 0$$

Balluffi, R. W.; Allen, S. M.; Carter, W. C. Kinetics of Materials; 1st ed. Wiley-Interscience, 2005.

Multiscale Modeling

- Thermodynamic free energy depends on the size of the sample
- Nonclassical thermodynamics
  - Free energy function depends on the gradient of order parameters

$$\text{¤} = \text{¤}\left(\text{¦}_i, \nabla \text{¦}_i\right)$$

Cahn, J. W.; Hilliard, J. E. The Journal of Chemical Physics 1958, 28, 258-267.

Lab instructions

- Cygwin
  - Follow the installation instruction at:

    http://rcc.its.psu.edu/user_guides/remote_display/cygwin/
- NX

  http://www.nomachine.com/download.php

Questions….