22.53 Overview

1. To understand the motivation and the basic purpose of this course, one might ask:
   - Why "statistical processes"?
   - Why "atomistic simulations"?
2. The aim is to **analyze** and **understand** complex phenomena, e.g., polymorphism, melting, amorphization or glass transition, plastic deformation and fracture - a host of microstructural processes in the case of materials applications. Other examples could be in fluid dynamics, biomolecular transport, etc.
3. Physical systems of interest tend to have many degrees of freedom (DOF), strongly coupled, and are usually **nonlinear**, **nonhomogeneous**, and **nonequilibrium**. They are difficult to study both theoretically and experimentally.
4. Partial answer to 1 above:
   - Systems which undergo strong fluctuations are best treated in statistical terms
   - Discrete-particle simulation provides the only tractable method of analysis.
5. An area of application of particular interest in this course is materials **modeling**, which is defined to be **theory and simulation**, combined with use of selected measurements for validation and parameterization.

   Why the special focus?
   - need for advance in fundamental understanding
   - exploit high performance computing (HPC)
   - emerging role of *computational* materials research, and increasing relevance of modeling across several length and time scales in a number of grand challenge-type initiatives launched by funding agencies

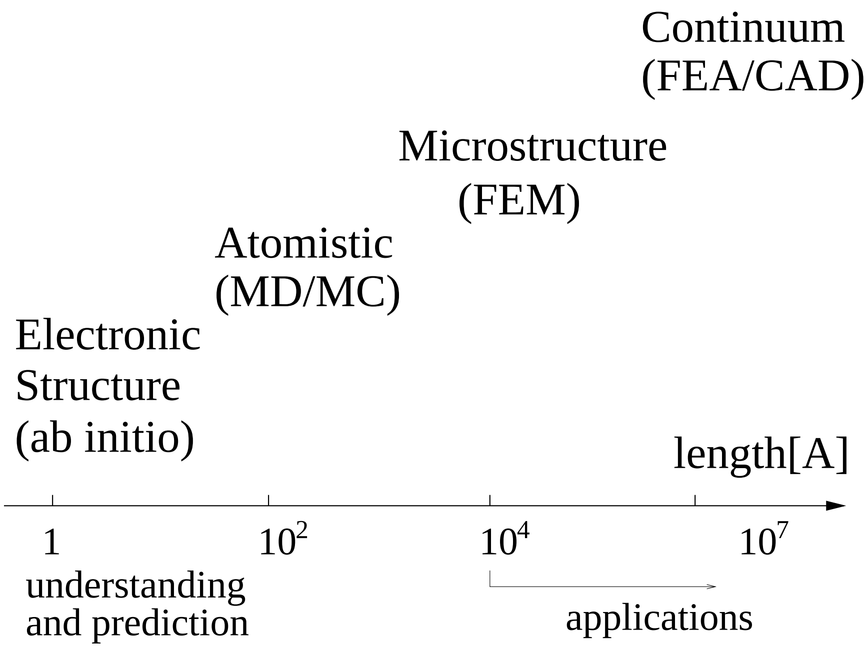

Figure 1: Four lengthscales in Multiscale Materials Modeling.

6. Multiscale Materials Modeling (MMM) - hierarchy of simulation techniques

   Fig. 1 shows the four lengthscales in MMM.

   - Electronic Structure
     - Quantum Chemistry
       - Hartree-Fock (HF) and Configuration Interaction (CI)
       - Coupled-Cluster and Many-Body Perturbation Theory
     - Density Functional Theory (DFT)
       - Local Density Approximation (LDA)
       - Generalized Gradient Approximation (GGA)
     - Local Combination of Atomic Orbitals (LCAO), also called Tight-Binding (TB): orthogonal vs non-orthogonal, selfconsistent vs non-selfconsistent.
   - Atomistic
     - Lattice calculations: cohesive energy, phonon dispersion curve, phonon Boltzmann equation, etc.
     - Static Minimization

    * Conjugate Gradient (CG)
    * Simulated Annealing
  - Molecular Dynamics (MD)
  - Monte Carlo (MC)
  - Quantum mechanical extensions such as Path Integral Monte Carlo (PIMC)
- Microstructural or Mesoscale
  - Kinetic Monte Carlo (KMC), a.k.a. Nodal Dynamics in dislocation context
  - Finite Element (FEM)
- Continuum
  - Finite Element Analysis / Computer Aided Design (FEA/CAD)
  - Computational Fluid Dynamics (CFD)

The final step is Product and Process Design, and of course, Marketing.

Note: applications lie mostly on the micron scale and above, whereas understanding and predictions normally occur at the molecular level and below. Effective linking of adjacent techniques is a major challenge.

A central theme across several lengthscales is **microstructure**, which can be as small as a point defect and as large as a visible crack on an airplane (see Fig. 2). Different microstructures interact in complicated manner depending on temperature, stress and chemical conditions. More often than not, *microstructures control the response of the material.*

7. In this course we will discuss primarily MD and MC. A simple definition is:

   each is a method of sampling the configuration of an N-particle system using specific interatomic interaction models

What are the frontiers? Materials modeling ...

Current developments: Workshop series ITP-UCSB '96 ... ASCI - Accelerated Strategic Computing Initiative ... SSI - Strategic Simulation Initiative ...

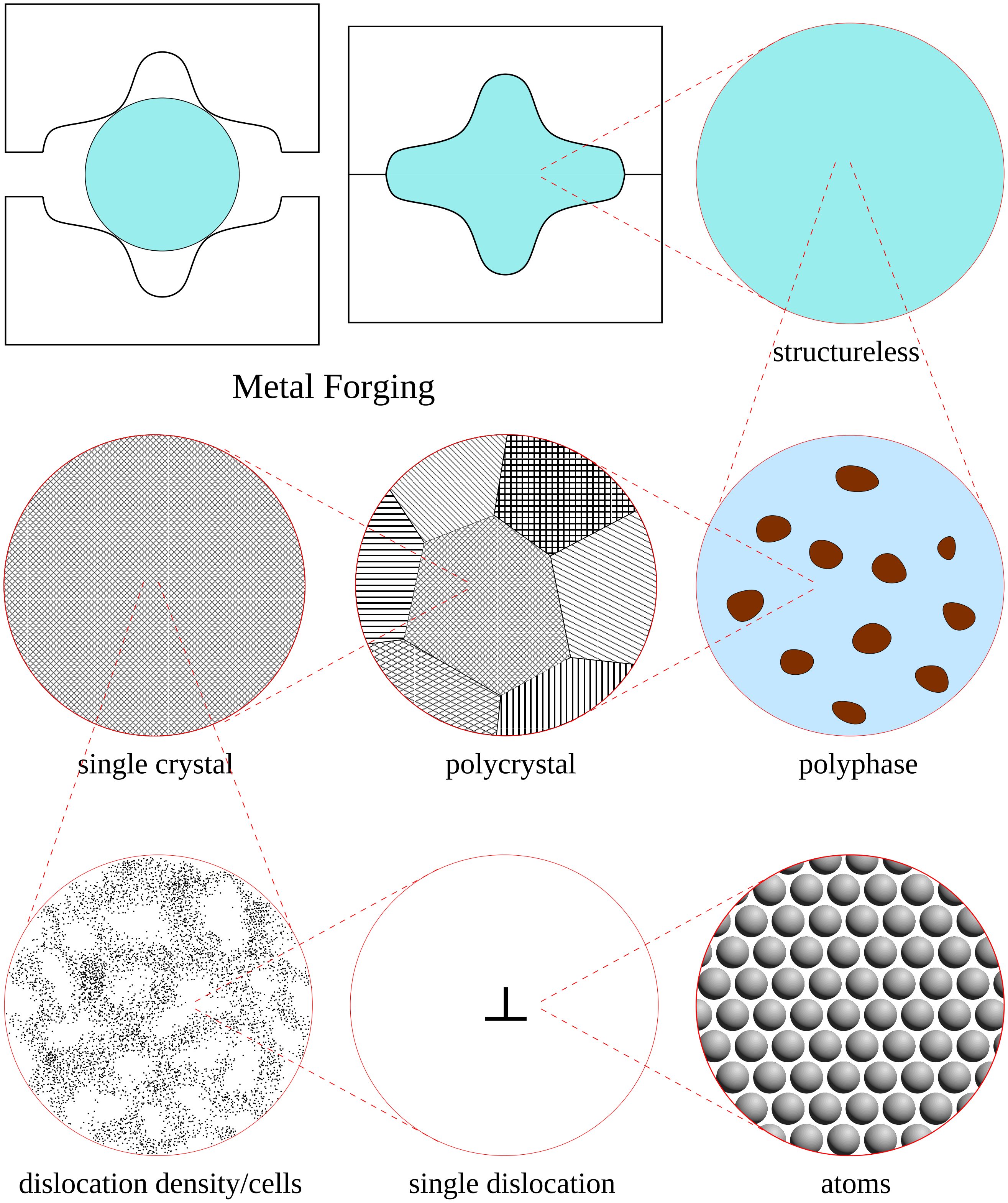

Figure 2: Microstructure across several lengthscales.

	MC	MD
driving factor for particle configuration change	potential energy	interatomic forces
type of dynamics	stochastic	Hamiltonian
type of sampling	probabilistic	deterministic
space sampled	configuration space $\{\mathbf{r}_1,..,\mathbf{r}_N\}$	phase space $\{(\mathbf{r}_1, \dot{\mathbf{r}}_1),.., (\mathbf{r}_N, \dot{\mathbf{r}}_N\}$

Table 1: Comparison of Molecular Dynamics (MD) and Monte Carlo (MC) methods.

Codes: - Haile [1], Li Ju, term project

References

[1] J.M. Haile, *Molecular Dynamics Simulation: Elementary Methods* (Wiley, New York, 1997).