Overview

- **Background, motivation, historical perspective, and biological relevance**

- **Molecular dynamics simulations in a nutshell, and its theoretical underpinnings**
  - Classical and statistical mechanical bases (integrators, ensembles, *etc.*)
  - Some algorithmic details
  - Strengths & weaknesses

- **MD in practice**
  - Force fields
  - Available software; pros & cons; how to do a simulation
  - Analysis of results – Basic ideas, what to look for, techniques, *etc.*
  - More recently developed MD-based methods (TMD, SMD, *etc.*)

- **MD applications & case studies**

  (1) structural biology (structure calculation and refinement), (2) drug design, (3) mechanistic enzymology, (4) "steered" MD investigations of myofibril elasticity

- **Current successes and near-term outlook**

Cameron Mura; May 2007