Short Course on Molecular Dynamics Simulation

Lecture 1:

Basic Concepts

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Course Objectives

- Awareness of the opportunities and limitations of MD simulation for scientific and engineering research
- Understanding of the compromise between model complexity/realism and computational expense
- Background that enables interpretation of MD studies reported in the literature
- Physical understanding of the theoretic basis of MD modeling

High Level Course Outline

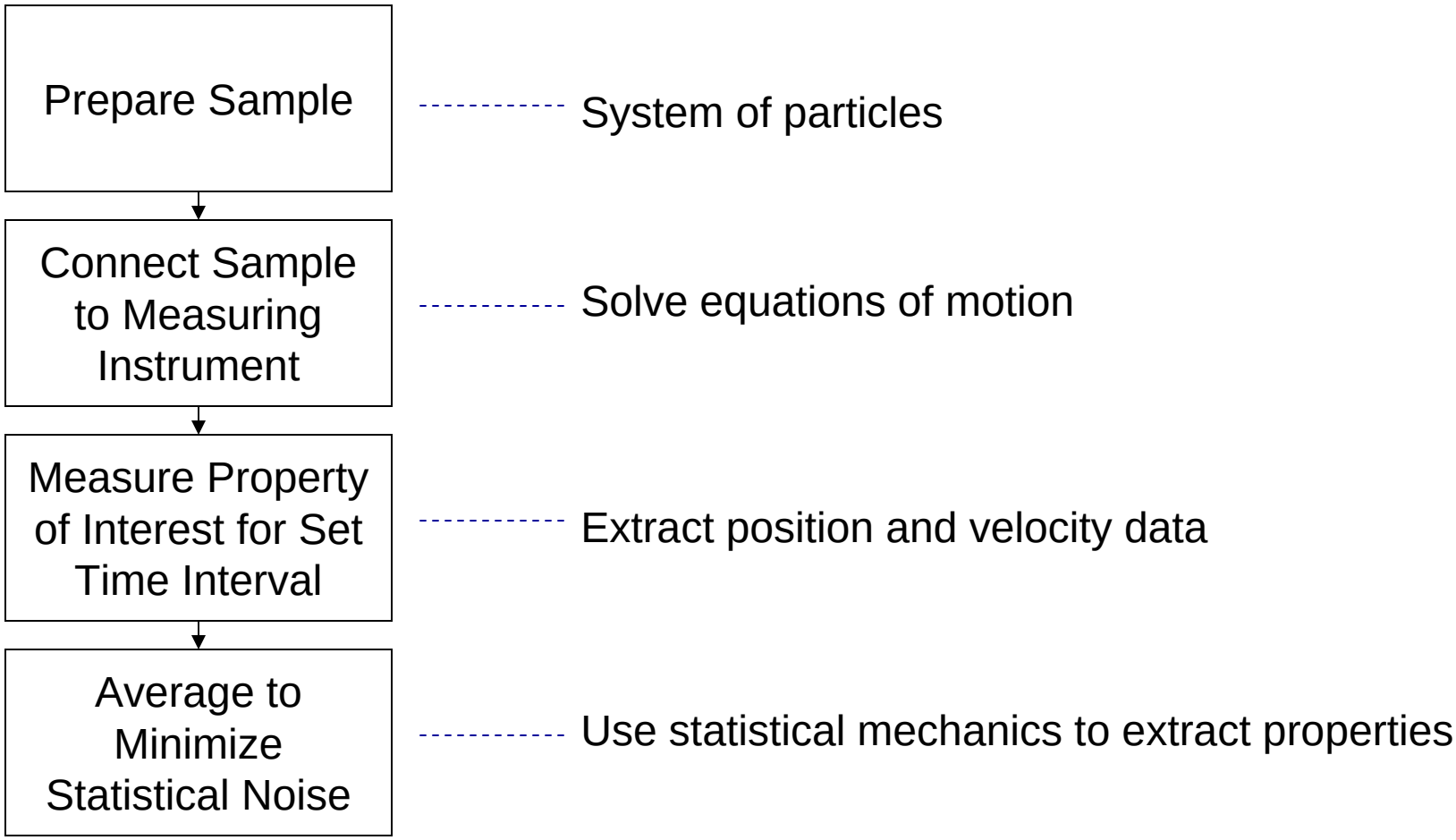
1. MD Basics
2. Potential Energy Functions
3. Integration Algorithms
4. Temperature Control
5. Boundary Conditions
6. Neighbor Lists
7. Initialization and Equilibrium
8. Extracting Static Properties
9. Extracting Dynamic Properties
10. Non-Equilibrium MD

MD Basics

- Molecular dynamics (MD) simulation = computational tool used to describe how positions, velocities, and orientations of molecules change over time.
- The simulation is based on a set of models that describe molecular-scale interactions.
- These models relate energy/force to configuration which are be used to calculate acceleration via Newton's law.
- Numerical integration yields particle velocities, and then each particle is moved through a distance equal to its calculated velocity multiplied by the simulation time step.
- So, MD is used as a computational "experiment" where a system is defined, allowed to evolve, and then observations made based on its evolution.

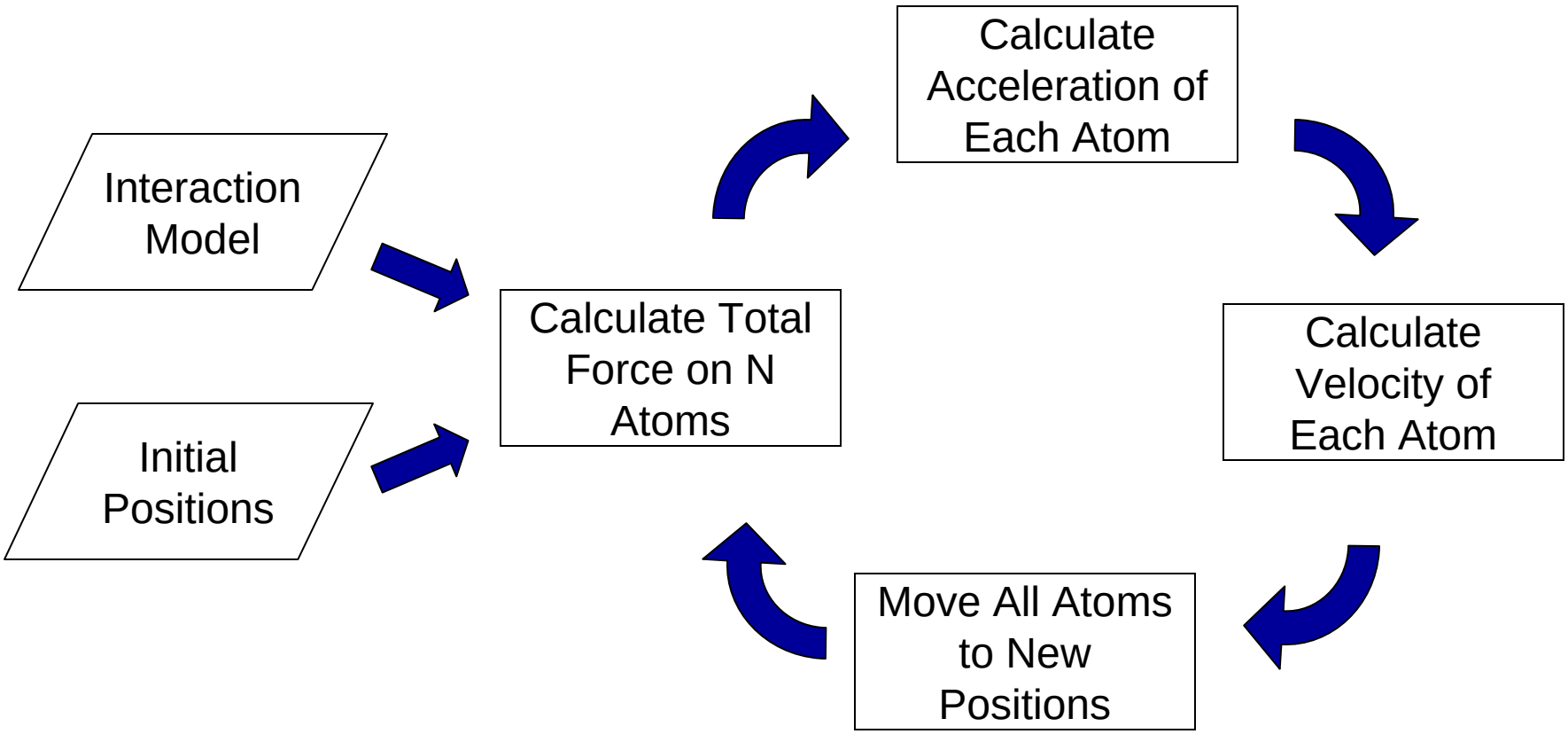
MD Basics

- Experiment
- MD Simulation



MD Basics

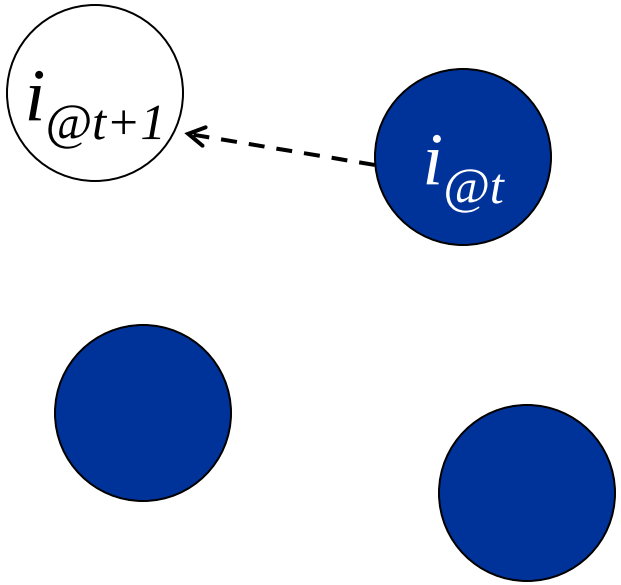
- Process summary



MD Basics

- Force → Acceleration → Velocity → Position

$$\vec{F}_i = m_i \vec{a}_i \qquad \vec{a}_i = \frac{d\vec{v}_i}{dt} \qquad \vec{v}_i = \frac{d\vec{r}_i}{dt}$$



Phase-Space and Ensembles

- MD conserves the total energy (Hamiltonian)

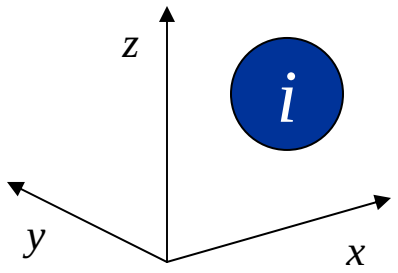
$$H(\vec{p}_i, \vec{r}_i) = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m_i} + U(\vec{r}_i) \qquad \frac{dH}{dt} = 0$$

KE

PE

Phase-Space and Ensembles

- A given atom is represented by its time-dependent position and momentum vectors

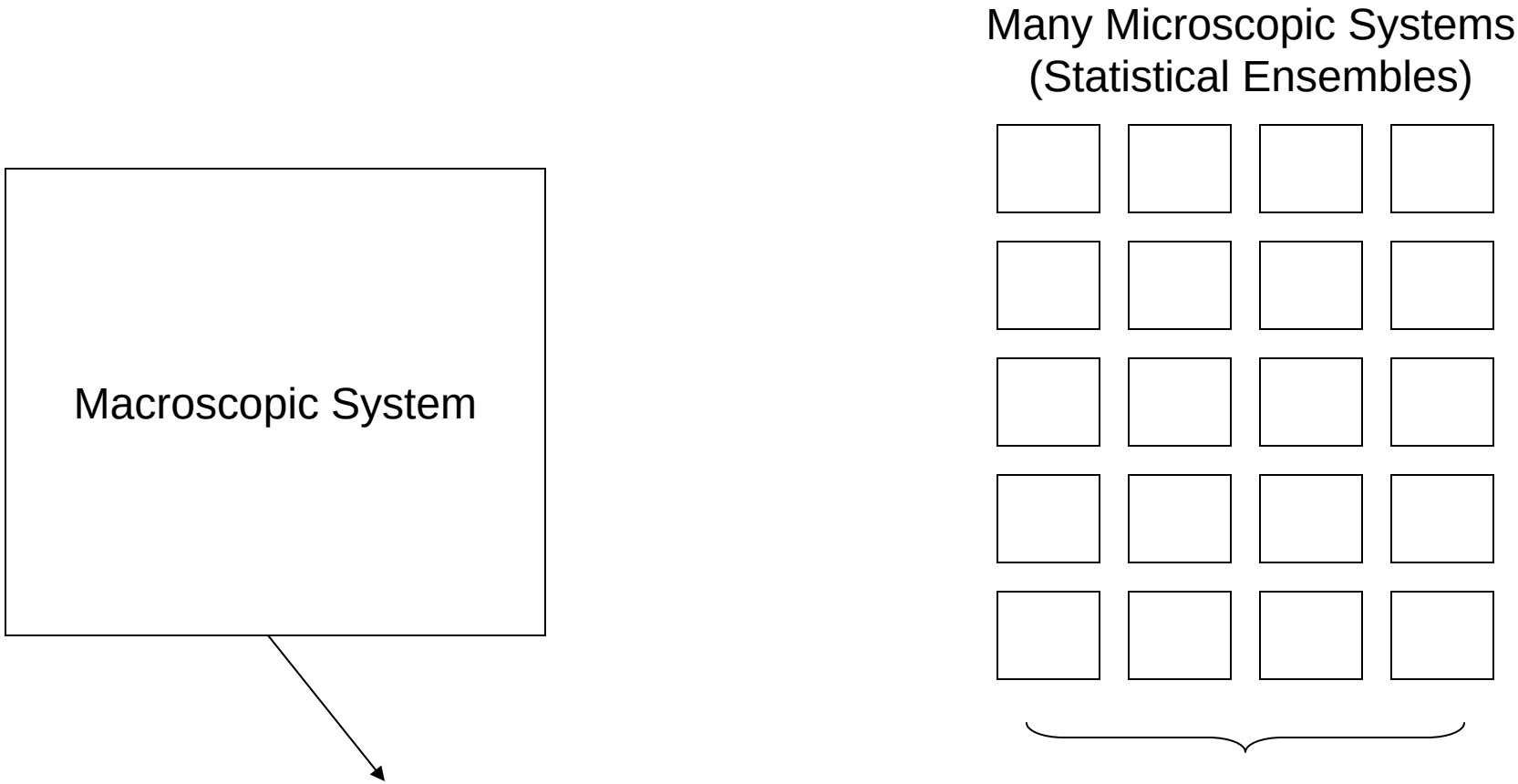


$$\vec{r}_i \qquad \vec{p}_i = m\vec{v}_i$$

- At a given instant, consider a plot of the positions and momenta of all N atoms in the system

6 N-dimensional plotting domain → Phase-Space

Phase-Space and Ensembles



Property of System = Average Property in all Systems
(Ensemble Average)

Phase-Space and Ensembles

- Ensembles characterized by fixed values of thermodynamic variables:
  - Energy
  - Temperature
  - Pressure
  - Volume
  - Number of particles
  - Chemical potential
- Basic MD – NVE
  - Micro-canonical ensemble
- Other common ensembles – NVT, NPT, μVT
  - Canonical, isothermal-isobaric, grand-canonical

References

- The following text books were used throughout the development of this course and should be used as references for in depth study
  - Allen, M.P and Tildesley, D.J., Computer Simulation of Liquids, Oxford University Press.
  - Frenkel, D. and Smit, B., Understanding Molecular Simulation: From Algorithms to Applications, Elsevier.
  - Haile, J.M., Molecular Dynamics Simulation: Elementary Methods, Wiley & Sons.
  - Leach, A., Molecular Modeling: Principles and Applications, Prentice Hall.