حسين التميمي

chapter two

Molecular dynamics

(Part 1)

Titles

2.1 Introduction

2.1.1 Atomic model in MD

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2.2.1 Pair potentials

2.2.2 Tersoff potential

Molecular dynamics

- Whether the famous apple actually fell on him or not, we will never know.
- Nevertheless(با این وجود) something opened Isaac Newton’s ingenious mind(ذهن نبوغانه) in 1686 to a new perception(درک) of nature and to conceive(فهم) the equations of motion.
- Mankind(بشر) seemed finally in a position to understand the rules of the game that nature played.
- The main equation describing this Newtonian world is as simple as

$$\boldsymbol{F} = m\boldsymbol{a} \tag{2.1}$$

where:

F is force vector
m is atomic mass
a is acceleration vector

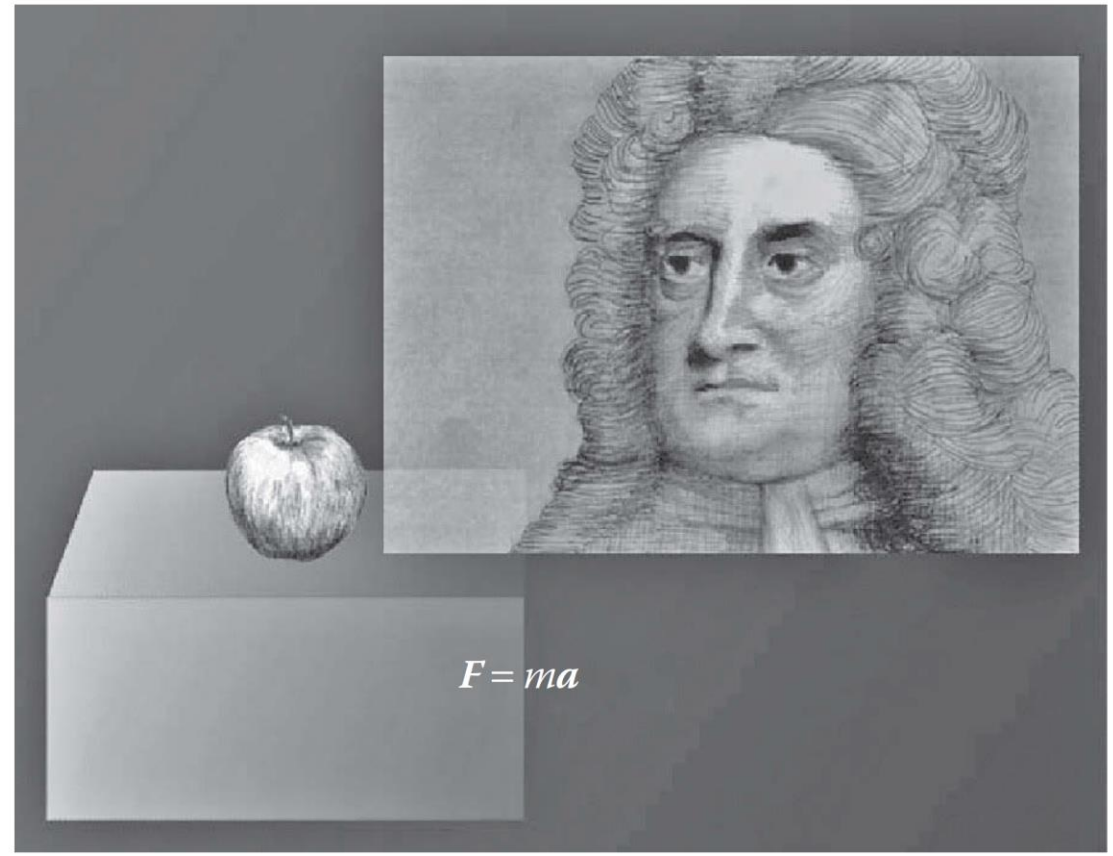

Figure 2.1 Sir Isaac Newton and the apple.

- The simple Equation 2.1 of three letters and a single mathematical symbol accurately predicted the motion of any particle-like objects: Newton's legendary(افسانه ای) apple, atoms, a flying baseball over the stadium, planets around the sun, and so on.
- The method using this classical mechanics for atomic movements is called molecular dynamics (MD).
- As the name indicates, it initially simulated a handful(تعداد انگشت شماری) of molecules but soon was extended to liquids, solids, and materials in parallel with the growth in computer power.

- In this chapter, by using atoms as the lowest level of information, MD will be treated(مورد عمل قرار گرفتن) for the predictions of static and dynamic properties of materials at the introductory level.
- For beginners, dealing with MD first will provide a smoother introduction to computational materials science because the subject is relatively easy and straightforward.
- With this knowledge on MD, we will be in a comfortable position to deal with first-principles methods in later chapters.
- Note that, however, MD has all the relevant basics for atomic-level resolutions(دقت) of materials by computation.

2.1 Introduction

- The primary goal of materials science is to improve existing materials and to design new materials.
- In computational materials science, we aim to achieve this goal by modeling and simulation.
- MD, the subject of this chapter, first started simulating just a bucketful(سطل) of hard spheres to see the liquid–solid phase transition (Alder and Wainwright 1957).
- Since then, efficient algorithms and powerful codes along with the ever-upgrading computing power have greatly accelerated the progress.

- A drastic(موثر) demonstration(نمایش) is the simulation of 320 billion atoms (Kadau et al. 2006).
- Although first- principles methods are becoming more and more popular these days, MD is still here to serve us where quantum effects are negligible.
- Recall that quantum effects become significant only when the particle wavelength, λ, is comparable with the interatomic distance (1–3Å). Otherwise, the use of the easier Newton's equations of motion is well justified.(مورد تایید است)

- Practically, MD is the only option for big systems of more than thousands of atoms.
- In this section, several essential topics for MD will be introduced before we solve Newton's equations of motion.

2.1.1 Atomic model in MD

- When we talk about gravity, matter as complex as Earth is often represented as a simple sphere even though we could describe it much better than that.
- We often present only the abstract instead of the whole paper, and it could still carry enough information to be useful.

- Approximation works the same way in computations, but only if we do it right.
- In MD, an atom is basically approximated as a sphere with point mass at the center as schematically drawn in Figure 2.2.

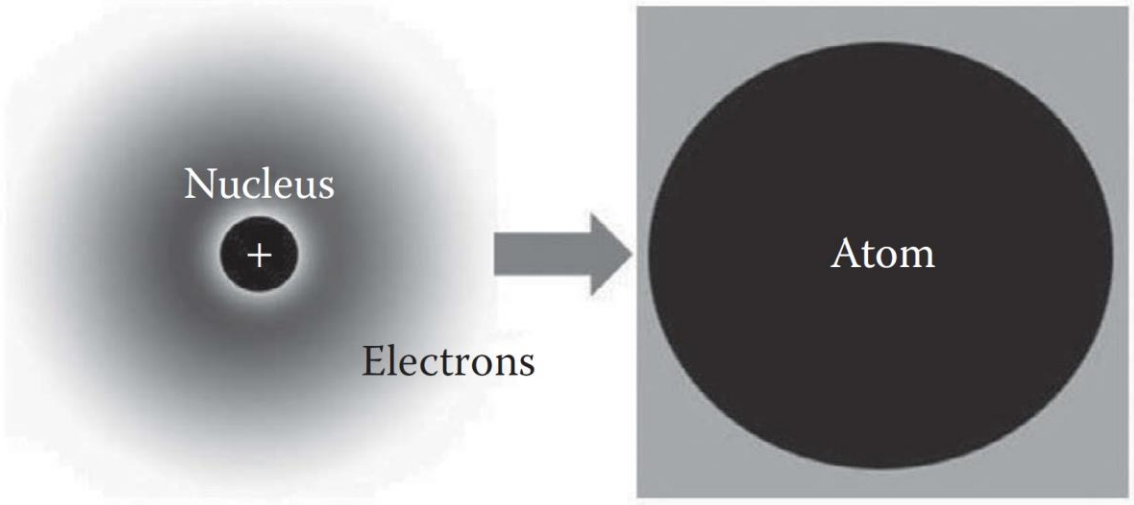

Figure 2.2 Schematic representation of atomic model in MD methods.

- This implies that the electron’s role is totally neglected.
- Thus, the computation becomes drastically simple because there is no need to do anything about electrons.
- There is, however, a negative consequence. Because of the presence of electrons, which is the origin of interatomic potential, is totally neglected, potential between atoms should be generated empirically to carry out MD.

2.1.3 Molecular dynamics

- MD is an integration of Newton's equations of motion over time to obtain the time evolution of the system and thus the properties of our interests.

- It generally proceeds as Figure 2.3b:

• Given the initial positions and velocities of every atom, and using the provided interatomic potential, the forces on each atom are calculated.

• Using this information, the initial positions are advanced toward lower energy states through a small time interval (called a timestep, Δt), resulting in new positions, velocities, and so on.

• With these new data as inputs, the above steps are repeated, typically for more than thousands of such timesteps until an equilibrium is reached, and the system properties do not change with time.

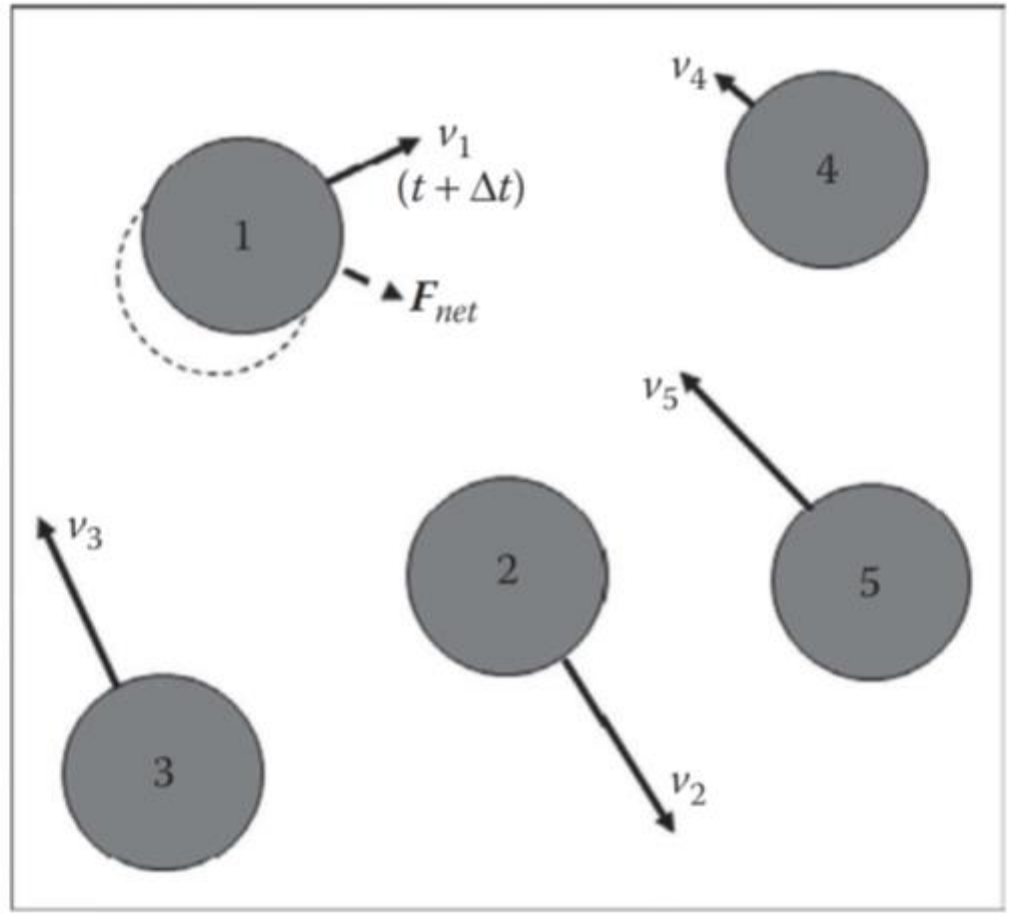

Figure 2.3

A typical procedures of MD in a five-atom system (#1 atom moved from the dotted-to the solid-ball position in Δt by the net force generated with other four atoms).

- During and after equilibration, various raw data are stored for each or some timesteps that include atomic positions and momenta, energies, forces, and so on.

- Properties that can be calculated directly or via statistical analysis from these data are as follows:

• Basic energetics, structural and mechanical properties.

• Thermal expansion coefficient and melting point.

• Heat capacity and thermal conductivity.

• Compared with the first-principles methods, MD is extremely fast and thus can handle much bigger systems. However, some limitations of MD include:

• Availability of potential is limited and the accuracy of a potential is always under question.

• Length scale is still not macroscopic, and time scale is also limited to nanoseconds.

• No electromagnetic properties can be obtained.