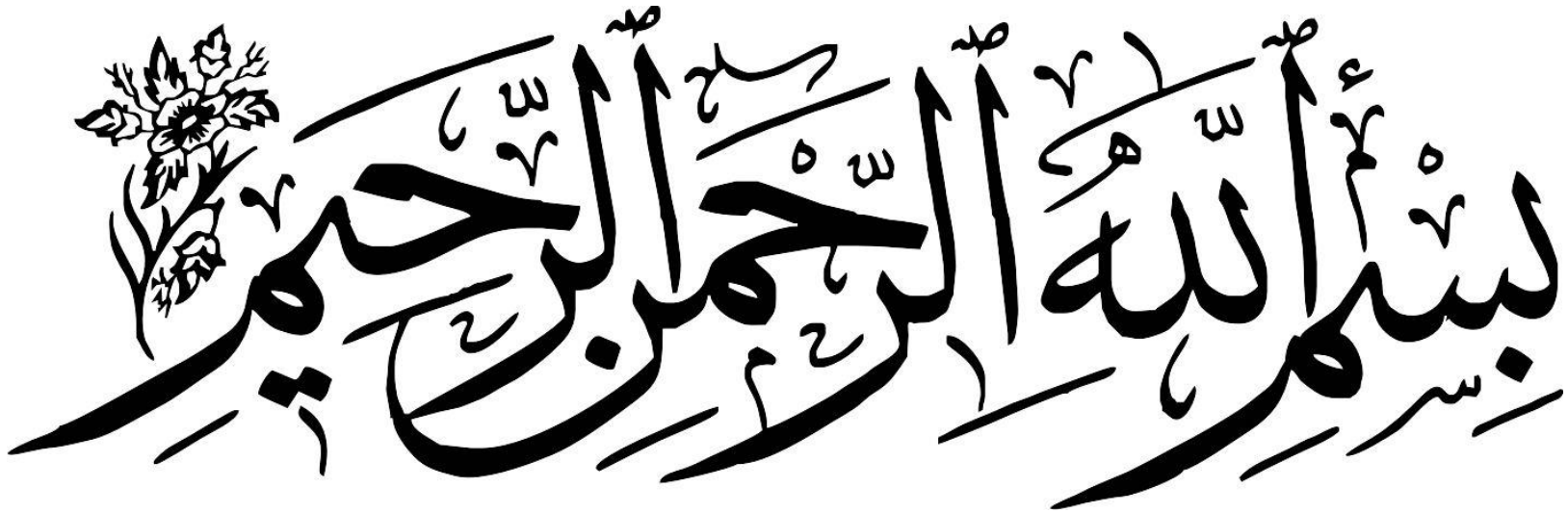
بسم الله الرحمن الرحيم

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1.1.1 Human beings versus matter

- We may say that we are all alike(مشابه) since all of us talk, work, play, and eat in a very similar manner. While this is true, our individual behaviors are so versatile(متنوع و مختلط) as a result of different feelings, ideologies(ایدئولوژی ها), philosophies, religions, and cultures that no individuals(هیچ کس) actually behave in exactly the same way.

- Despite scientific studies on human behaviors and mental(ذهنی) processes, it is very difficult to predict events that involve humans. we cannot even tell whether the person next to us will stand up or remain seated in the very next moment.

- On the contrary, atoms and their constituting electrons and nuclei (the main characters at the arena(حوزه) of computational materials science) always follow specific rules without exceptions.
- If an exception is observed, it is more likely that it is a mistake due to a human error. Unlike humans, an electron never kills itself or other electrons because of love.
- The same goes for nuclei, atoms, molecules, and materials. They simply follow the known laws of nature, which are mainly classical and quantum mechanics in terms of electromagnetic force .
- Therefore, we can foresee(پیش بینی) practically all forms of phenomena encountered(موجود) in materials by tracing down the interactions between them.

1.1.2 Computational materials science

1.1.2.1 Goals

- In computational materials science, we aim to understand various properties and phenomena of materials and achieve designing and making better materials for society. This goal is realized by modeling materials with computers that are programmed with theories and algorithms based on physics, mathematics, chemistry, material science, and computer science.
- For example, the sintering(پختن) behavior of a metal or a ceramic can be normally studied with the usual sintering furnace(کوره) in a laboratory. However, it can be done on a computer by using molecular dynamics (MD) on atomic scale. By changing various input conditions, the entire spectra of data can be generated efficiently and accurately if the runs are set up properly.

- In many cases, a computational approach may become the only way to handle materials under extreme conditions that can never be reached in a laboratory: under high pressures, at high temperatures, and in the presence of toxic substances or nuclear radiation.
- For example, the materials under nuclear fusion((fission:شکافت)همجوشی) environments are of great concern(نگرانی) these days.
- The various damages occurring in fusion materials by neutron irradiation can be simulated without worrying about expensive(گران) equipment(تجهیزات) and danger of radiation.

- Let us look at another example that has great impact on our daily lives.
- Every day we use a cell phone, smart phone, smart pad, TV, computer, and so on, which employ IC chips usually made of silicon. Using computational materials science, we can design better materials and develop faster, smaller, and lighter IC chips.
- To summarize, there is no doubt that computational materials science will change the paradigm(الگو) of materials research. It will change “lab experiments” with heavy equipment to “keyboard science” on computers.
- Currently, computational materials science is no longer(نیست ... دیگر) a specialized topic(موضوع تخصصی). It has become familiar and routine such as analyzing XRD curves and examining SEM or TEM images.
- Furthermore, most people recognize that computational materials science is not just an optional topic but an essential one. It is not surprising to hear scientists say “computation first, then experiment” or “material design by computation.”

1.1.2.2 Our approach

- I wrote the following comparison as an illustration in my book (Lee 2003) published in 2003, but allow me to restate it. For a materials scientist, computational science is a convenient(راحت) tool such as a car.
- In order to operate a car, it is not necessary to understand how the engine block is cast(قالب بندی) with molten(مذاب) metal or how the combustion(احتراق) energy transfers from engine to wheels as the mechanical energy of rotation.
- We only need to know how to use the accelerator, brakes(ترمزها), and steering wheel(فرمان), as well as be aware of a few traffic rules. Then, we check the car for maintenance(تعمیر) if we notice anything wrong.

- Similarly, we use computational methods with well-proven(ثابت شده) codes, run it, obtain data, and check the results with experts(کارشناسان) if we find something amiss(خطا و اشتباه).
- It is not necessary to understand all the theories, algorithms, and equations in detail.
- It is also not necessary to understand the codes or programs down to the bits and bytes. This knowledge is reserved for other professional physicists and chemists.

1.2 Methods in computational materials science

In this section, the basic procedures and methods in computational materials science are briefly introduced.

1.2.1 Basic procedures of computational materials science

- If matter is affected in any way(به هر حال) in this world, we can safely say that it is a result of one of the four known fundamental interactions: electromagnetic, strong nuclear, weak nuclear, and gravitational. Fortunately(خوشبختانه), as far as(تا آنجایی که) materials science is concerned(مربوط), we need to consider only the electromagnetic interaction; we rarely encounter cases with the other three.

❖Thus, what happens in any materials in any circumstance is narrowed down to the electromagnetic interactions between nuclei, electrons, and atoms.

❖ Based on this simple fact, the basic procedures of computational materials science may be stated as follows:

• Define what to calculate.

• Make a model system that represents the real system properly.

• Select the relevant rules (classical mechanics, quantum mechanics, theories, algorithms, etc.).

• Select a code/module/program/package to do the job for the system.

• Run simulation, analyze the results, and refine(تصحیح کردن) the run under better-defined conditions.

• Produce data and compare them with reported data by other relevant studies and experiments.

- In short, we are recreating a part of nature in the frame of our simulation system in a simplified and well-controlled manner.
- Among these steps, the last should not be underestimated(دست کم گرفتن). The simulation results is derived from somewhat(تا حدی) idealized situations and therefore must be critically(انتقادی) examined using experimental data.
- In the following subsections, the four typical methods for performing the above-mentioned processes are briefly outlined.
- As shown in Figure 1.4, all four methods have advantages and limitations in terms of system size and simulation time. Multiscale methods, which combine two or more methods, are also included in the figure.

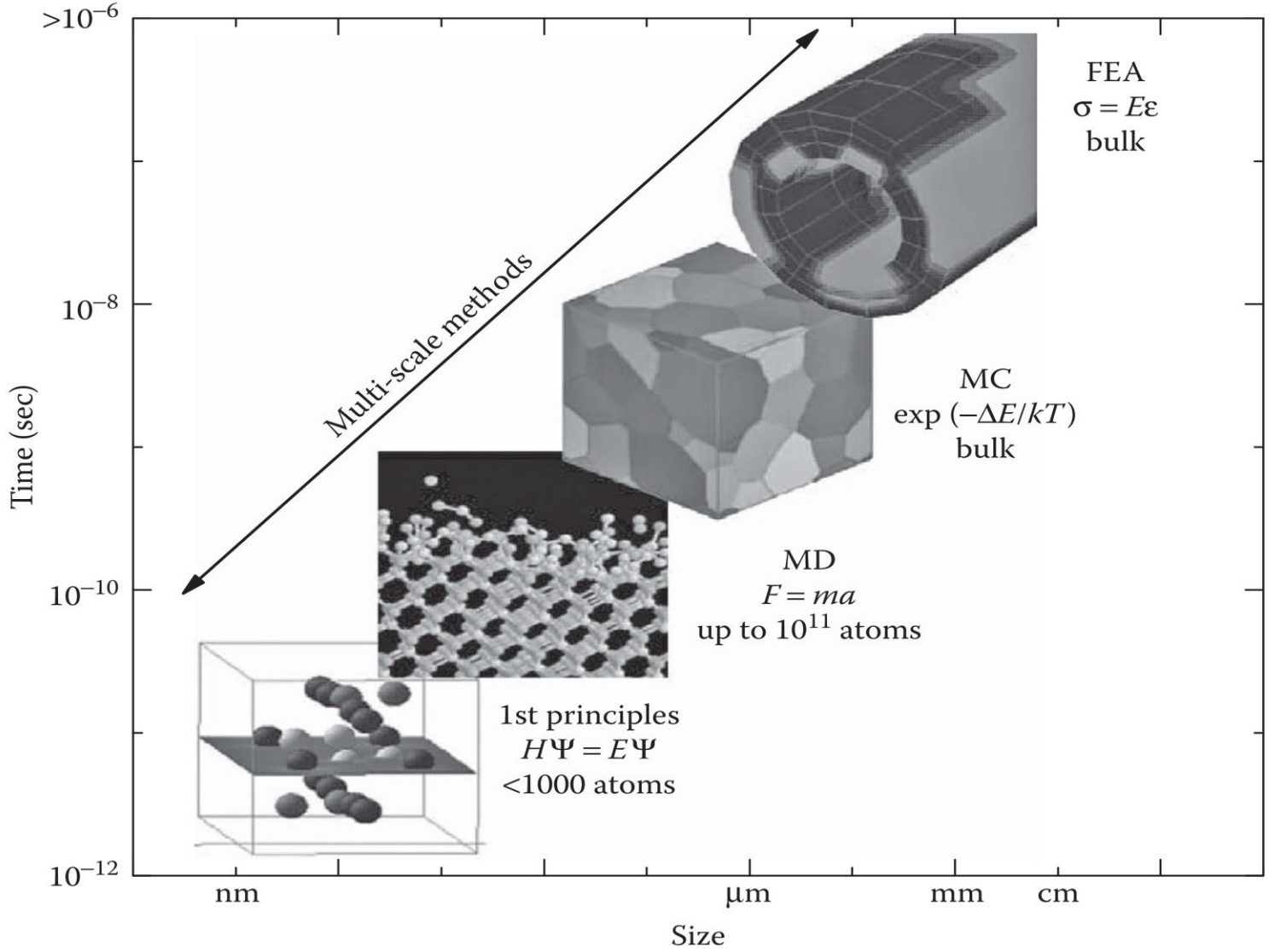

Figure 1.4 Typical methods in computational materials science in terms of size and time.

1.2.2 Finite element analysis

- Finite element analysis (FEA) involves dividing the system into many small elements and calculating variables such as stress, strain, temperature, and pressure.
- Sets of algebraic, differential, and integral equations are solved by a computer-based numerical technique.
- This method provides solutions to a wide variety of complex engineering problems including materials properties and phenomena (elastic and plastic deformation, fracture, heat transfer, etc.) for the scale of real components(اجزا).

1.2.3 Monte Carlo method

- The Monte Carlo (MC) method is a statistical technique that involves using discrete and random walks(روشهای) for sampling(نمونه گیری) and the Boltzmann factor of $\exp(U/k_BT)$ for probability to solve problems in materials and many other systems. Here, U is the energy of a state, k_B is the Boltzmann constant, and T is temperature.
- The method is conceptually very simple and easy to implement since it simply lets the atoms jump around randomly and picks the lowest energy state.
- It can equilibrate any degree of freedom, and no dynamics is needed since it is based on statistical mechanics.
- The scale of the MC method is in microns and can thus treat microstructures of materials.

1.2.4 Molecular dynamics

- MD considers atoms as the basic particles and disregards nuclei or electrons.
- Therefore, the system can be well described classically by using Newton's equations of motion that involve relatively easy differential equations for only atom–atom interactions.
- In the 1960s, only several hundreds of atoms were simulated by MD, but the number of atoms has increased to more than 100 billion these days.
- The catch is that(نتیجه این است) we have to empirically generate the interacting potential between atoms since the origins of potentials (nuclei and electrons) are completely excluded in this method. For the same reason, electronic and magnetic properties cannot be obtained.
- Once the potential is known and the initial positions and velocities are given, the time-evolutions of the atoms can be revealed in a rather straightforward fashion(روش).

1.2.5 First-principles methods (ab initio methods)

- The first-principles methods consider nuclei and electrons as the basic particles and describe events in a subatomic world.
- The system, therefore, can be expressed only by quantum mechanics that involves relatively difficult partial differential equations.
- In the 1930s, only simple hydrogen like atoms were calculated by quantum mechanical methods, but now the number of atoms has increased to over several thousands by the advent(با ظهور) of density functional theory (DFT).
- All properties including electronic and magnetic ones can be obtained given that(با توجه به اینکه) nuclei and electrons are considered in the method.