

بِسْمِ اللَّهِ الرَّحْمَنِ الرَّحِيمِ



عنوان درس:

فیزیک محاسباتی سیستمهای نانومتری

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# Introduction

Reference: [Computational Materials Science AN INTRODUCTION](#)

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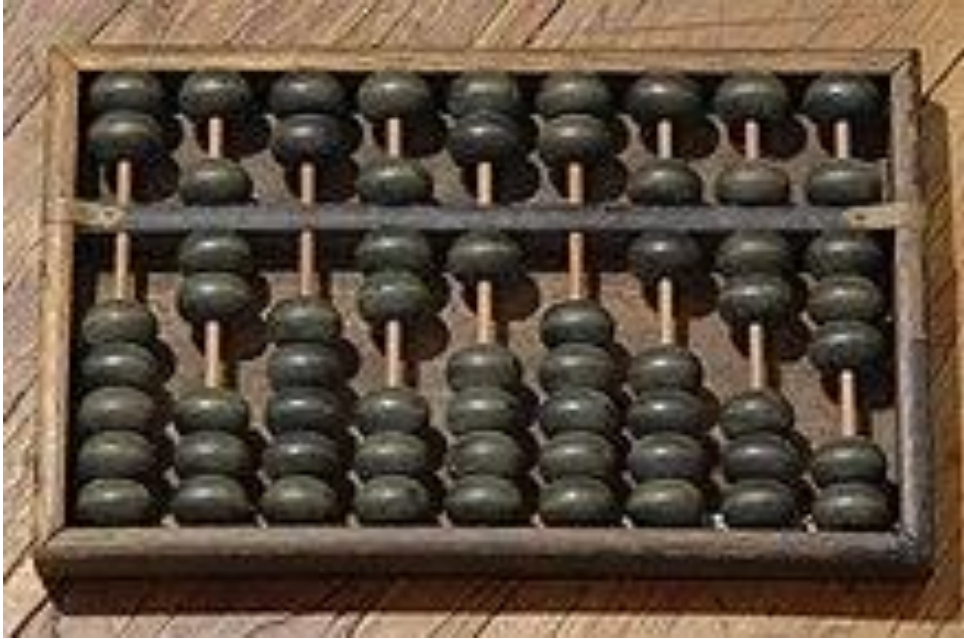
# Preface (پیشگفتار)

- ❖ No longer underestimated (غیر قابل انکار است), computational science has emerged as a powerful partner to experimental and theoretical studies.
- ❖ Accelerated by the ever-growing power of computers and new computational methods, it is one of the fastest growing fields in science these days.
- ❖ Its predictive (پیش بینی) power in atomic and subatomic scales benefits (فایده رساندن) all disciplines (رشته ها) of science, and materials science is definitely (قطعاً) one of them.
- ❖ Note that, for example, materials under extreme conditions such as high temperature or pressure, high radiation, on a very small scale, can be rather easily examined via the keyboard in computational materials science.

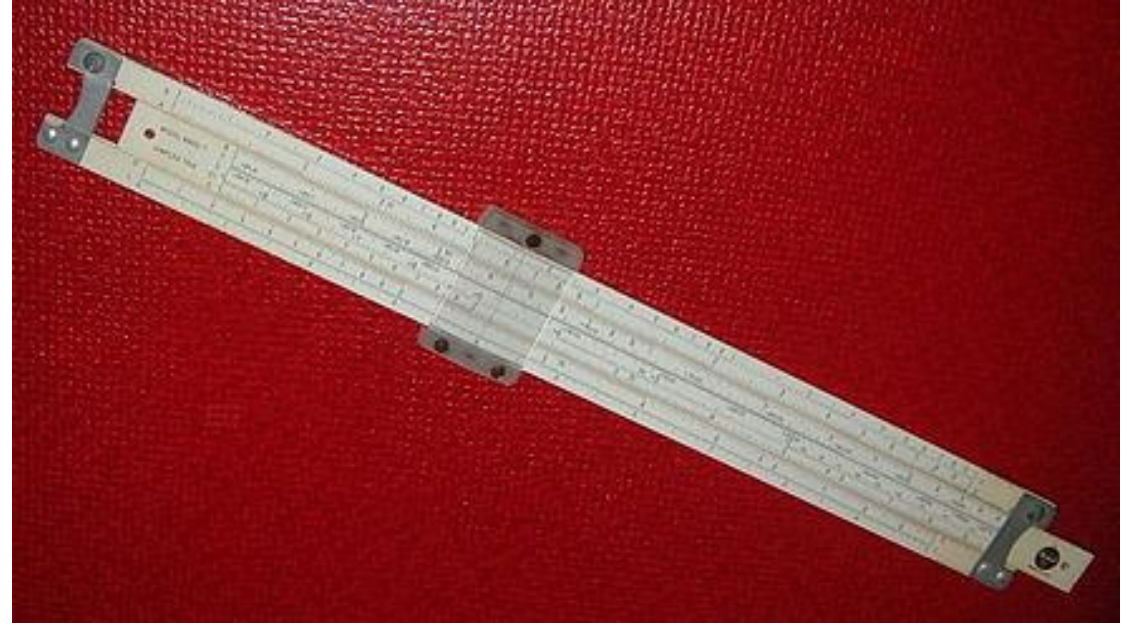
- ❖ Computational science has been a familiar subject in physics and chemistry, but in the materials field it was considered of secondary importance.
- ❖ A materials system may be described at three different levels: the electronic structure level of nuclei and electrons, the atomistic or molecular level, and the finite element level of coupled structural elements.
- ❖ With these tools, we simply try to bring a very small part of nature on computer as a system, and apply the known rules of nature to solve a certain problem.

# Introduction

- ❖ It is amazing how much computing power has progressed since the invention of the Chinese abacus: from slide rule to mechanical calculator, vacuum-tube computer, punch-card computer, personal computer, supercomputer.

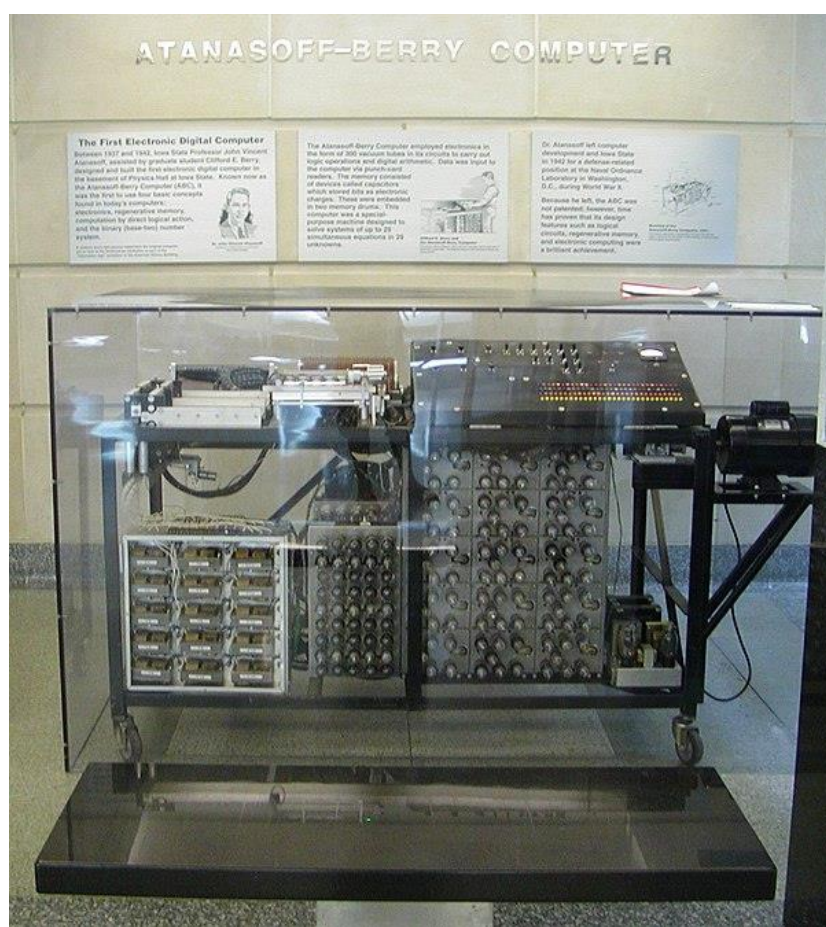


Chinese abacus

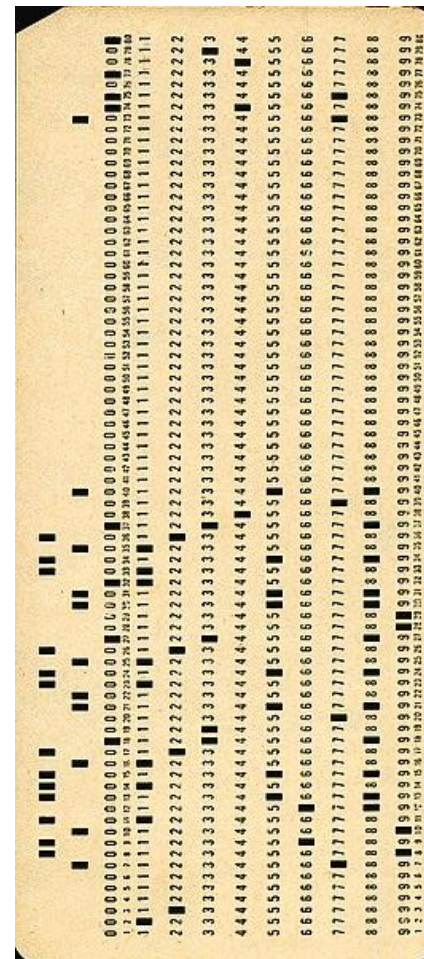


The slide rule is a mechanical analog computer. The slide rule is used primarily for multiplication and division, and also for functions such as exponents, roots, logarithms. Though similar in name and appearance to a standard ruler, the slide rule is not meant to be used for measuring length or drawing straight lines.





A vacuum tube computer, now termed a first-generation computer, is a computer that uses vacuum tubes for logic circuitry. Although superseded by second generation, transistorized computers, vacuum tube computers continued to be built into the 1960s.



A punched card is a piece of stiff paper that can be used to contain digital data represented by the presence or absence of holes in predefined positions.





A personal computer (PC) is a multi-purpose computer whose size, capabilities, and price make it feasible for individual use. Personal computers are intended to be operated directly by an end user, rather than by a computer expert or technician.



A supercomputer is a computer with a high level of performance as compared to a general-purpose computer.

- ↓ ❖ Calculation speed has increased roughly  $10^{10}$  times in the span(محدوده) of about 50 years and is still growing. Its immense(شگرف) impact on every sector(بخش) of society is astonishing(عجیب).
- ❖ In this chapter, the significance of computational science in materials is addressed, and a brief description of the various methods is presented.