CSE115:Introduction to Biology and Chemistry for Computation

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Lecture Outline

- Introduction
- Computer for Chemistry
- Computer for Biology
- Future scopes

Introduction

- We live in the era of computers. The word computer comes from the word “compute”, which means, “to calculate”. Despite computing it has many aspects in our life.
- The evolution of computer is still on and the ability of computers to sort massive amount of data and quickly produce useful information for almost any kind of user, makes them essential tool in modern society.

Fields of Computer

- Science(e.g. Chemical industry)
- Medicine(e.g. Bioinformatics)
- Education
- Banking
- Crime Investigation
- Entertainment
- And much more

Computers in Chemistry :

- There are several scopes of working for computer engineers in chemistry. Such as:
- **Computational chemistry**
- It is the branch of chemistry where computers are used for solving chemical problems related to simulation. It uses methods of theoretical chemistry, incorporated into computer programs, to calculate the structures and properties of molecules, groups of molecules, and solids

Visual Models & Packages

- Many self-sufficient computational chemistry software packages exist. Some include many methods covering a wide range, while others concentrate on a very specific range or even on one method.
- For example:
  - For drawing packages -*ISIS/Draw by MDL* Information Systems
  - For modelling packages such as *ArgusLab*
  - These software packages allow you to create your own molecular-structure

Applications of computer for chemistry in Industry

- **DCS (distributed control system)**
- A distributed control system (DCS) is **a** computerized control system for a process or plant usually with many control loops

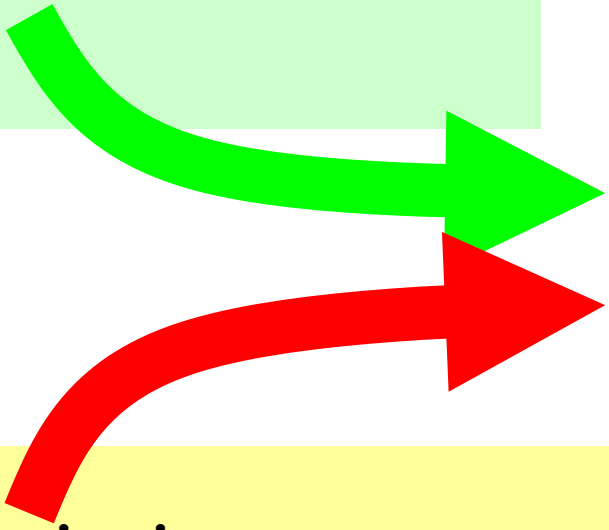
- **Chromatography**
- Chromatography is an analytical technique commonly used for separating a mixture of chemical substances into its individual components

Computers in Biology :

- Computer has worked wonderfully in Medical science and biology. There are numerous of fields in biology where computer has successfully proved it's existence.
- **Bioinformatics:**
- Bioinformatics is the interdisciplinary field where computer science, mathematics, physics, and biology are merged.

The field of science in which **biology**, **computer science** and **information technology** merge into a single discipline

Biologists
collect molecular data:
DNA & Protein sequences,
gene expression, etc.



Bioinformaticians
Study biological questions by analyzing molecular data

Computer scientists
(+Mathematicians, Statisticians, etc.)
Develop tools, softwares, algorithms
to store and analyze the data.

Computers in Biology

- DNA sequencing
- Sequence Alignment
- Gene duplication
- DNA database searching
- Gene Therapy
- Drug development


QUESTIONS