

Computational modeling can be a useful partner in biotechnology, in particular, in nanodevice engineering. Such modeling guides development through nanoscale views of biomolecules and devices not available through experimental imaging methods.

We illustrate the role of computational modeling, mainly of molecular dynamics, through four case studies:

Development of silicon bio nanodevices for single molecule electrical recording, development of carbon nano-tube-biomolecular systems as in vivo sensors, development of lipoprotein nanodiscs for assays of single membrane proteins, and engineering of oxygen tolerance into the enzyme hydrogenase for photosynthetic hydrogen gas production.

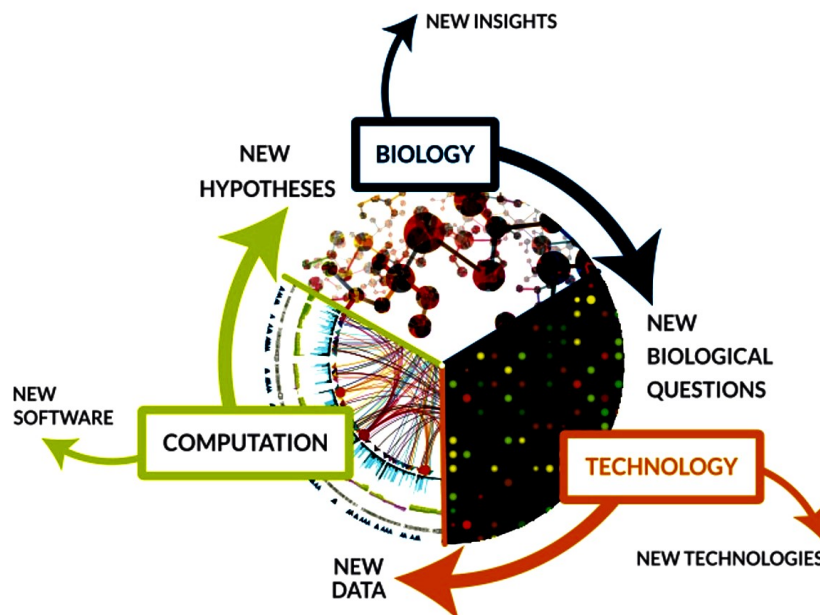
The four case studies show how molecular dynamics approaches were adapted to the specific technical uses through (i) multi-scale extensions,

(ii) fast quantum chemical force field evaluation,

(iii) coarse graining,

(iv) novel sampling methods.

The adapted molecular dynamics simulations provided key information on device behavior and revealed development opportunities, arguing that the "computational microscope" is an indispensable nanoengineering tool.



## **Bioinformatics Engineers**

Bioinformatics Engineers, also called Bioinformatics Software Developers, are computer scientists that write software applications and tools that are used by biologists in the field of biotechnology and bioinformatics to perform research and analysis.

Bioinformatics engineering requires deep understanding and sound knowledge of algorithms, data structures, high performance computing, and software engineering. These are wholly or partly covered in the field of computer science. Moreover, before a person can be a bioinformatics engineer, they must have sound programming skills.

A typical bioinformatics engineer in **Seres Therapeutics**, Cambridge (MA), designs, models, and develops data management systems that integrate lab, operation and research data. The job requires that the bioinformatics engineer be qualified in computer science and some other related disciplines. Bioinformatics engineers also design and maintain high performance biological data pipelines that can be used by biologists.

## **Computational Biologists**

The job of a computational biologist is sometimes erroneously thought to be the same as that of a pharmaceutical scientist. However, though they do overlap somewhat, computational biology is different. It is a job that requires the combination of computer science and biology to develop the underlying algorithms that are used in data analysis to try and understand biological processes. In modern society, biological and genetic data are much more accessible.

As a result, skilled computer scientists are relied on to use computational processes to find solutions to problems such as genetic disorders, diseases, and other problems. This is because computer programs can be used in a wide variety of ways in science, for example in hypothesis testing and tracking causation. Thus biologists no longer work alone. Computation is now an integral part of biological experiments and assays.

Therefore, biotechnology companies are now integrating computer science professionals with biologists to apply the best possible computational methods and concepts to the biological data in order to advance scientific knowledge.

## **Bioinformatics Analysts**

Bioinformatics Analysts perform large scale analysis and manipulation of biological data in order to present the data in an organized way

These analysts take huge chunks of biological data and process them through computer programs (developed by computational biologists), create models, and perform statistical analyses to generate insights from the data. Bioinformatics Analysts work closely with biologists; they also can work with Bioinformatics Engineers to provide requirements for data processing systems, visualization methods, and user interfaces that can be used by large teams.

A typical Bioinformatics Analyst at Translational Genetics for Regeneron Pharmaceuticals, New York, provides bioinformatics support for genetics projects and manipulates genotypic and phenotypic data to support Regeneron's research and developmental activities.

Computer science jobs are very relevant in the field of biotechnology and the computer science skills will continue to be crucial to the growth of the field.