UNIVERSITÀ DEGLI STUDI DI MILANO

Structural Bioinformatics

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Time table

Tuesday 14.30-17.30: Computer room at the Department of Biosciences, if you have never been there, go before the next week to register an account (if you want to use the local machines).

Friday 13.30-15.30: room 501 (ISU)

Course Material

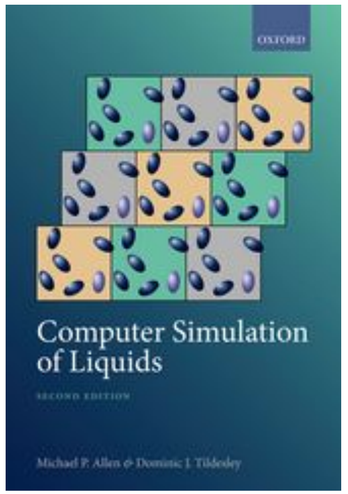
Most material is available from GitHub:

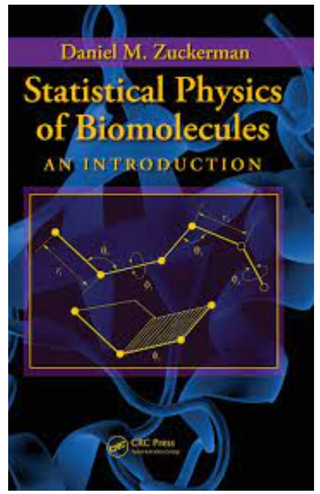
https://github.com/carlocamilloni/Structural-Bioinformatics

- Slides

- Review papers provided

All this material is part of the EXAM





Exam

Produce reports for all the lab experiences: one/two of them will be discussed at the exam

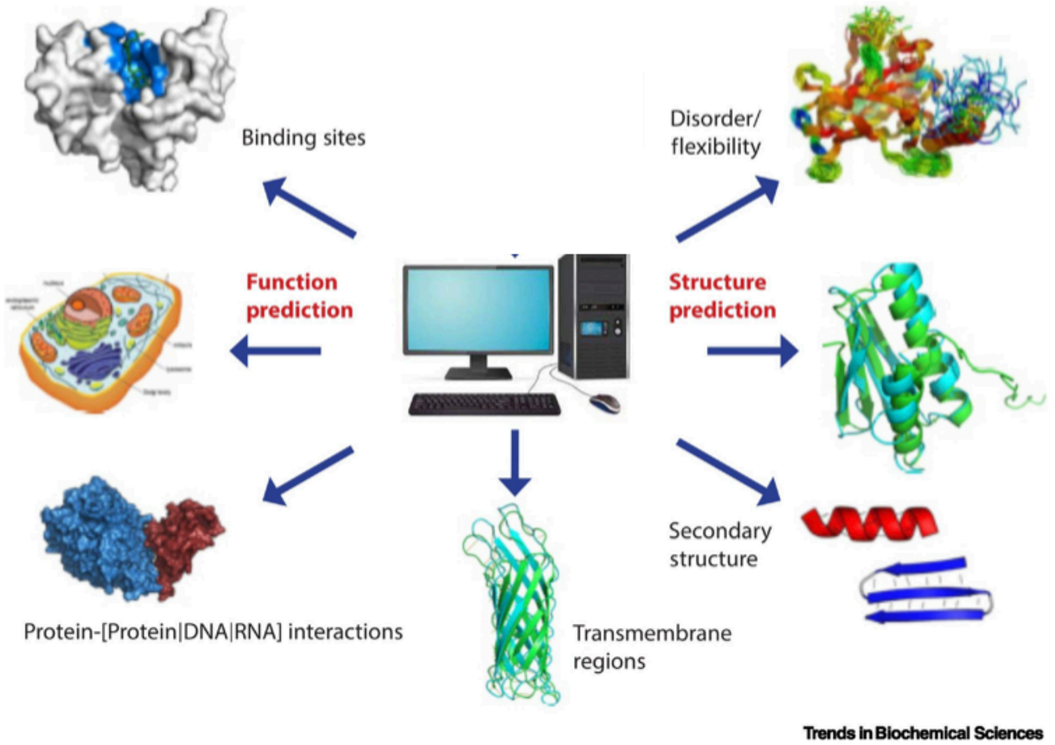
Make a presentation (~10 min) to discuss a scientific paper from a list I will share at the end of the course. Most questions will be on those techniques employed in the paper you chose and that have been presented in the lectures.

Structural Bioinformatics

Nowadays SB covers a number of different topics that involve the structure of biomolecules and the use of computers to study them:

- How to predict the structure of biomolecules (proteins, but also nucleic acids, complexes, etc.)
- How to study their function and/or disfunction including the effect of mutations, partners, environment
- How to design new biomolecules

SB inherits from statistical methods, physics, chemistry, biochemistry and structural biology.



Bordin, N. *et al*. Novel machine learning approaches revolutionize protein knowledge. *Trends Biochem. Sci.* **48**, 345–359 (2023).

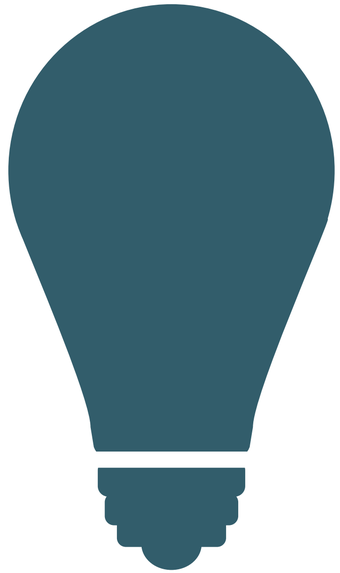
Aims and Background

- **Have a general understanding of what you can do with computer modelling (what kind of problems can be addressed and how?)**

- **Have a general understanding of the theoretical concepts that are the foundation of the field (why things work?)**

- **Know what are the strengths and weaknesses of different methodologies (What is the right method for a given problem and what are the limitations?)**

- **Have the tools to read and understand the scientific literature of the field**



Program

1. **Statistical Picture of Biomolecules: theoretical framework**
2. **Structural Biology and Visualisation**
3. **Classical Molecular Dynamics**
4. **Enhanced Sampling Techniques**
5. **Markov State Models**
6. **Quantum Chemistry and Simplified Models**
7. **Machine Learning**
8. **Structure Prediction and Molecular Docking**
9. **Integrative Modelling and Protein Design**

Topics will be both introduced theoretically and tried hands-on doing guided exercises

Practicals

Install VMD (version 1.9.4) if you will use your own laptop

https://www.ks.uiuc.edu/Research/vmd/

We are going to use COLAB: colab.research.google.com

To use them (essentially to save the results of your work)
You need a google Drive account, please do one

You can work alone or in small groups (two/three).

Reports should be produced summarising all activities