Practical Aspects in Computational Biophysics

IF PAN - Spring 2023
Course Description
Dr. Paweł Krupa

1 Overview

Who? When? Where?
Class: Mondays 13:00 - 15:00 (first lecture: Feb 27)
Location of lectures: Zoom
Lecturer: Paweł Krupa
Email: pkrupa@ifpan.edu.pl
Office: 100 building VIII IF PAN
Office hours: Mondays 15:00-16:00

Course Description:
The course will focus on practical aspects of conducting scientific studies in the field of computational biophysics and similar areas. Each lecture (except the first one, which will be a brief introduction of the methods) will contain hands-on examples on how to use popular methods, tools, and servers and which options/parameters are the most critical to ensure high quality of the results.

Prerequisites:
A basic background in statistical physics, computational biophysics and programming would be helpful but not necessary.

Textbook:
This will be a practical research-driven course. Students will receive appropriate lecture notes and relevant references for further reading/practicing.

Evaluation:
It will be based on engagement and a presentation during the course.

2 Syllabus

Class number	Date	Subject
1	Feb 27th	Introduction to popular methods used in computational biophysics: all-atom and coarse-grained force fields, molecular dynamics (MD) and Monte Carlo simulations, molecular docking, structure prediction, etc.
2	Mar 6th	CHARMM-GUI - preparation of the input files for various biomacromolecular systems and methods.
3	Mar 13th	Running of MD simulations in an all-atom Amber force field (minimization, equilibration, periodic boundary conditions, different ensembles, conventional and enhanced sampling MD runs, etc.).

4	Mar 20th	Running of MD simulations in coarse-grained models (SIRAH, Martini, UNRES) and methods to speed-up calculations - part one.
5	Mar 27th	Running of MD simulations in coarse-grained models (SIRAH, Martini, UNRES) and methods to speed-up calculations - part two.
6	Apr 3rd	Running non-standard simulations (SMD, umbrella sampling, PMF, with ligand parameterization, with 12-6-4 potential).
7	Apr 10th	Holidays
8	Apr 17rd	Popular methods and servers to run MD simulations, molecular docking, and analysis.
9	Apr 24rd	Methods and servers to predict protein, protein-protein, protein-ligand structure and estimate the quality of the prediction.
10	May 1st	Holidays
11	May 8th	How to combine chemoinformatics, bioinformatics, and machine learning with computational biophysics.
12	May 15th	Analysis and visualization of the data - build-in and in-house made tools (Gnuplot, Python, Shell scripts, cpptraj etc.).
13	May 22th	Searching for data: how to find and read the best publication and the most important information to verify the study/plan the experiment.
14	May 29th	Writing a scientific document (manuscript/PhD thesis) (LaTeX, MS Word, Google Docs, etc.) with use of citation managers (EndNote, Mendeley, PaperPile, BibTeX, etc.) and online and offline platforms.
15	June 6th	Summary and conclusions of the lecture.