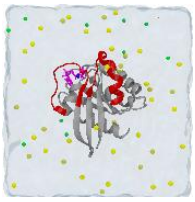

Hands-on Molecular Dynamics Workshop

6 April 2019, 09:00-17:00
Department of Physics, Faculty of Science, Birzeit University
Room 016

Background: Predicting the effects of, e.g., a mutation or a change in the pH on the structure, dynamics and function of a protein is possible thanks to molecular dynamics simulations. Anyone with basic molecular biology and physics background and a general interest in computer simulations can setup and run computational modeling and dynamics experiments.

Objectives: Participants will use popular open source tools and techniques necessary for conducting successful molecular dynamics experiments.

Who should attend: Researchers and students interested in learning tools to explore, visualize and understand biomolecular structures and their functions in three dimensions.

Who will teach: Members of the Palestinian-German Science Bridge (PGSB)

- Mrs. Hebah Fatafta, Forschungszentrum Jülich
- Dr. Abdallah Sayyed Ahmad, Birzeit University
- Dr. Thorsten Auth, ICS-2, Forschungszentrum Jülich
- Prof. Birgit Strodel, ICS-6, Forschungszentrum Jülich

Schedule:

09:00 - 10:30 Introduction

- General Introduction about the workshop and computational biophysics (Mrs. Fatafta + Prof. Sayyed Ahmad)
- Introduction to PGSB, Forschungszentrum Jülich and IHRS BioSoft (Dr. Auth)
- Introduction to Dr. Auth's research (Dr. Auth)
- Introduction to Prof. Strodel's research and molecular dynamics (MD) simulations

10:45-11:55: Hands-On morning session

- Basic Linux commands
- Visualization of proteins with VMD

12:00-12:50 Lunch Break

13:00 - 17:00 Hands-On afternoon session

- Setting up and running an MD simulation
- Analysis of MD simulations