UNIVERSITY of MISKOLC
Faculty of Materials and Chemical Engineering

Antal Kerpely Doctoral School of Materials Science & Technology

Computational Biochemistry

Dr. Michael C. OWEN

COURSE DESCRIPTION

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Computational Biochemistry

Dr. Michael C. OWEN

Lecturer

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Recommendation

The lecture is proposed for all students of the Kerpely Doctoral School, with a special focus on students interested in chemistry and computer simulations.

Language

English.

Scope

The main goal of the course is to provide students with an overview of modern molecular dynamic (MD) simulation tools and apply them to biopolymers, condensed phases and biological macromolecules.

Methodology

The course is conducted through in-person lectures and practical sessions. The lectures and practices are structured to provide a comprehensive understanding of simulation methods. Students are then trained to apply these methods to the GROMACS software package, enabling them to apply their knowledge practically to systems of interest.

Topics

1. Introduction to MD Simulations.
2. Applications of MD within the GROMACS software package.
3. MD Simulations of Proteins and Biopolymers.
4. MD Simulations of Condensed Phases.
5. Applications of Advanced Sampling Techniques.

References

1. M.J. Abraham, T. Murtola, R. Schulz, S. Páll, J.C. Smith, B. Hess, and E. Lindahl, "GROMACS: High performance molecular simulations through multi-level parallelism from laptops to supercomputers," SoftwareX, 1–2 19–25 (2015)
2. Frenkel, D. and Smit, B. (2002) Understanding Molecular Simulations. 2nd Edition, Academic Press, San Diego.
3. M.J. Abraham, D. van der Spoel, E. Lindahl, B. Hess, and the GROMACS development team, GROMACS User Manual version 2018, www.gromacs.org (2018)

Exam

Project work.

Complex exam questions

1. Explain what is the simulation box and its requirements. What are periodic boundary conditions? What is its purpose? What are its considerations with respect to the molecules in MD simulations?

2. Explain four limitations or approximations used in MD simulations.

3. Explain how proteins are polymers. How can the study of proteins translate to the structure and properties of polymers? Give specific examples.

4. What is a potential energy surface? Use a diagram and an example in your explanation.

5. Explain what is the simulation box and its requirements. What are periodic boundary conditions? What is its purpose? What are its considerations with respect to the molecules in MD simulations?