Advanced Hands-On Module: Introduction to Molecular Dynamics Simulations with Classical, Atomistic Force Fields

Summer 2022

Particle-based molecular dynamics (MD) simulations are a method to numerically solve Newton's equations of motion, thus propagating in time the position of each particle in a system. Molecular dynamics simulations where the interactions between each atom are represented using simple potential energy functions ("force fields") and where covalent bonds cannot be broken or formed are appropriate to investigate a range of equilibrium and non-equilibrium physical-chemical phenomena. This type of simulations have yielded unprecedented insight into the structure, dynamics, interaction mechanisms, transport mechanisms in liquids, soft matter and biological systems. E.g., MD simulations have clarified the molecular mechanism of the rotation of water molecules, the structure of the air-water interface, the mechanical deformation of proteins to applied force, the mechanisms of interaction of peptides with phospholipid membranes or the mechanisms of ion transport across ion channels in cell membranes. MD simulations can be analyzed at the single-molecule level, providing a timeline of the response of individual molecules with femtosecond resolution that is often impossible to get from experiment. At the same time, observables can also be spatially and/or temporally averaged for direct comparison with the outcomes of typical experiments. This workshop will consist of an introduction to MD simulations. The course will include an overview of the basic principles of MD using classical potentials to describe interatomic interactions, followed by a practical session during which students will set up a short simulation of a biological system and will analyze its results. There are no prerequisites. The goal is to give you a foundation that enables you: to critically read published simulation studies of interest for your own work, to assess which of your research questions could be usefully investigated using this technique, and to set up simple simulations.

Venue: University of Duisburg-Essen, MG building - Room 382, Lotharstr. 1, 47057 Duisburg
Duration of the course: 10th June, 2022 from 09:00am-05:00pm.
Maximum number of participants: 4

Contact id: hosein.daronkola@uni-due.de; ana.araujo-vila-verde@uni-due.de