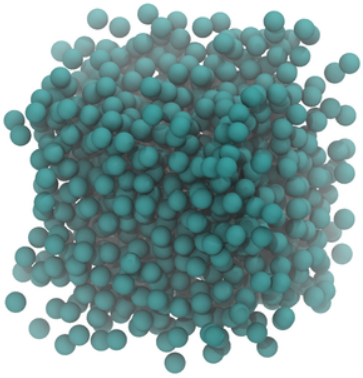
Universidad Nacional de Córdoba

UNICAMP

Sep. 5th to 9th, 2022
2 pm to 4 pm



COMPUTING THERMOPHYSICAL PROPERTIES OF FLUIDS USING MOLECULAR DYNAMICS SIMULATIONS

This is an introductory hands-on course on the molecular dynamics (MD) simulations. The main goal is to show how one can compute thermophysical properties of fluid systems using molecular dynamics simulations. In particular, we will use GROMACS, a free and open-source code, that can handle very large simulations in a very efficient way. We will discuss the role of force fields in these calculations, as well as the variety of existing force fields for different applications. We will study the fundamental concepts underlying the computation technique such as: the Verlet algorithms for numerical integration of the classical equations of motion, periodic boundary conditions and the minimum image convention, long-range corrections to pressure and to energy, and the use of thermostats and barostats for NPT simulations. In terms of the thermophysical properties, we will apply MD simulations to compute:

- density,
- heat capacities,
- diffusion coefficient,
- and viscosity

Dr. Luís Fernando Mercier Franco

is currently an Associate Professor at the School of Chemical Engineering of the University of Campinas, Brazil. He obtained his D.Sc. in chemical engineering from the University of São Paulo, Brazil, under the supervision of Prof. Pedro de Alcântara Pessoa Filho, with part of his D.Sc. being developed in the group of Prof. Edward Maginn at the University of Notre Dame, USA. In 2015, he received the Helmut Knapp Award at the European Symposium of Applied Thermodynamics held in Athens, Greece. In 2016, he moved to Qatar as a Postdoctoral Research Associate in the group of Prof. Ioannis G. Economou at Texas A&M University at Qatar. His research focuses on the chemical engineering application of classical thermodynamics, statistical mechanics, and molecular simulation.