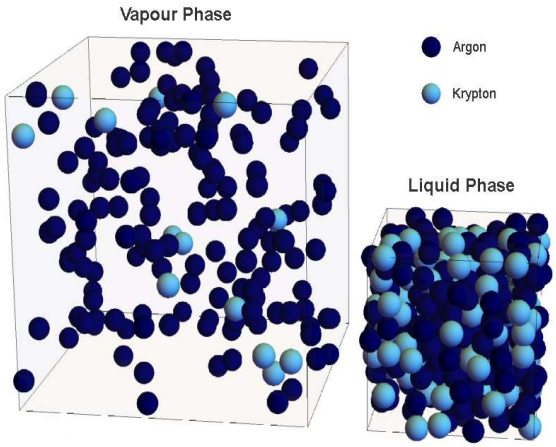
Monte-Carlo Simulations

Topic suitable for Bachelor Thesis



This research topic, providing several BSc theses, is based on the application of our recently published and constantly updated molecular simulation suite implemented in Wolfram Mathematica [1]. This package provides a so-called Gibbs-Ensemble Monte-Carlo (GEMC) simulation environment that is predestined for the determination of fluid phase equilibria, like vapor-liquid (VLE).

The aim is to simulate selected systems, e.g. the homologous series of n-alkanes, alcohols and mixtures thereof, and to assess the simulation results by comparison with data from literature and/or equations of state.

This includes the parameterization of the molecules, the collection of experimental data from literature for comparison, conducting the simulations and assessment of the results.

Selected parts of the simulation results will serve as input for an upcoming research project.

Literature:

[1] Wolfram Notebook Archive: Gibbs Ensemble Monte Carlo Sim. for Fluid Phase Equilibria. https://notebookarchive.org/2022-11-6ger7tx

Assoc.Prof. Thomas Wallek (thomas.wallek@tugraz.at)