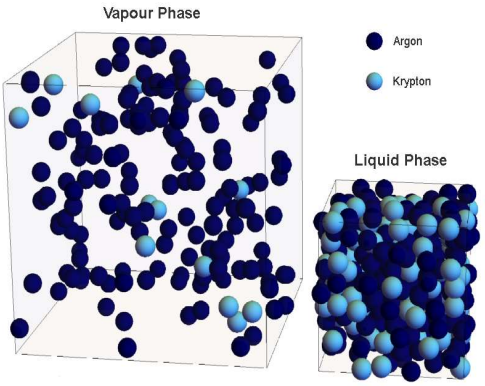
Gibbs-Ensemble Monte-Carlo Simulation

Topic suitable for Bachelor Thesis / Plant Design



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 thesis aims at the simulation of VLE for selected molecules, to explore and optimize the related simulation strategies. This happens in each case with increasing complexity, starting with a simple Lennard-Jones sphere model and ending with a polyatomic molecule. Simulation strategies are assessed by comparison of the simulation results with data from literature and/or equations of state. For operating the well-documented simulation package, a basic understanding of Wolfram Mathematica concepts is required, e.g., by exploring the interactive website http://www.wolfram.com/wolfram-u/an-elementary-introduction-to-the-wolfram-language/.

Literature:

[1] https://notebookarchive.org/2022-11-6ger7tx The Wolfram Foundation Notebook Archive.

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