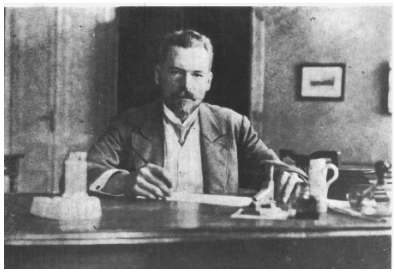

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Monte Carlo simulations of liquid crystal phases: behind the scenes

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Computer simulations are a basic tool for modeling soft matter since only a handful of models can be solved exactly or they can be treated only with phenomenological theories. For most soft interactions a standard molecular dynamic (MD) integration is a go-to tool. However, hard interactions pose a problem because of infinite forces during collisions. While there exist collision event-driven extensions to MD, the most straightforward way of simulating hard-core systems is the Monte Carlo Metropolis-Hasting algorithm. Although the basic version of the Monte-Carlo (MC) algorithm is easy to implement, it becomes very inefficient for a large number of interaction centers. This work summarizes some optimizations, including neighbor grid and parallelization using domain division which enables to simulate tens of thousands of interaction centers for tens of millions of full MC cycles within a reasonable time. Moreover, it provides a summary of problems that may hinder the equilibration of the system together with possible solutions to them.

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