# What can go wrong when computer simulations applied outside their original context

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In an article about to be published in *European Physical Journal Plus*, Daan Frenkel from the University of Cambridge, UK, outlines the many pitfalls associated with simulation methods such as Monte Carlo algorithms or other commonly used molecular dynamics approaches.

The context of this paper is the exponential development of computing power in the past 60 years, estimated to have increased by a factor of 10152, in line with Moore's law. Today, short simulations can reproduce a system the size of a bacterium.

The author singlehandedly outlines diverse examples of issues arising when seemingly simple simulation methods are not applied with the due level of care. For example, simulations of small-scale systems, such as cubic boxes representing a unit cell as part of a crystal or liquid crystal, display effects that are linked to the fact that the sample is of finite size. Therefore, these simulations can only imitate, not reproduce, macroscopic effects unless effects that occur at microscopic scale, such as surface effects, are effectively removed. This is typically done by using periodic repetition of a small system in all directions.

Frenkel also focuses on methods that, at first blush, appear reasonable, but are flawed and are akin to attempting to compare apples and oranges. For example, computing a mechanical property of a system—say the potential energy—using a Monte Carlo simulation, which can be based

on thermal averages, does not allow us to compute the thermal properties of such a system—such as entropy—in terms of thermal averages. Finally, the article also takes great care to debunk common myths and misconceptions pertaining to simulations, for instance, newer simulation methods are not necessarily better than older ones.

**More information:** D. Frenkel, Simulations: The dark side, *European Physical Journal Plus*, DOI 10.1140/epjp/i2013-13010-8

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