From a model of fluids to the birth of a new field in computational physics

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It may sound like the stuff of fairy tales, but in the 1950s two numerical models initially developed as a pet project by physicists led to the birth of an entirely new field of physics: computational statistical mechanics. This story has recently appeared in a paper published in *EPJ H*, authored by Michel Mareschal, an Emeritus Professor of Physics at the Free University of Brussels, Belgium.

The article outlines the long journey leading to the acceptance of such models—namely Monte Carlo and Molecular Dynamics simulations—as reliable evidence for describing matter. This happened at a time when the computing power required to run simulations was scarce. Today, these techniques are used by thousands of researchers to model the behaviour of materials, in contexts ranging from fusion to biological systems.

The saga began in 1951, when John G. Kirkwood from the California Institute of Technology, USA, developed this counter-intuitive theoretical prediction: a model of hard spheres—a rough model for any fluid— undergoes a transition from a fluid to a solid state under controlled conditions. This implies that the ordered solid form holds more entropy—or has more space available for moving around—than the disordered fluid form. These spheres do not normally interact with one another, like molecules in a perfect gas—experiencing an infinite repulsion when they come into contact.

Kirkwood's theoretical prediction remained controversial until it was

supplemented by intensive parallel work pursued by two teams of US physicists, originally launched as side projects. The first involved Bill Wood at the Los Alamos Laboratory, and led to the development of the Monte Carlo approach; the second, which involved Berni Alder at Livermore National Laboratory, led to the development of molecular dynamics. Ultimately, it was the introduction of importance sampling—a clever way to perform Monte Carlo—on the part of Marshall Rosenbluth (also at Los Alamos) that proved to be a real stroke of genius in confirming Kirkwood's prediction.

More information: Michel Mareschal, Early years of Computational Statistical Mechanics, *The European Physical Journal H* (2018). DOI: 10.1140/epjh/e2018-90006-7

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