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CREATED BY PREDICTION: ON THE HISTORY, ONTOLOGY, AND COMPUTATION OF THE LENNARD-JONES FLUID

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ABSTRACT

The Lennard-Jones (LJ) fluid, named after mathematician-physicist-chemist Sir John Lennard-Jones (1894-1954), occupies a special place among fluids. It is an ideal entity, defined as the fluid whose particles interact according to the Lennard-Jones potential. This potential describes the pairwise repelling (very small distance) and attracting (van der Waals) forces with a relatively simple and mathematically tractable expression.

The contribution discusses the history of the LJ fluid in four acts. Act one starts with classical mechanics and leads to the early 20th century when theoreticians like Mie, London, and Lennard-Jones combined available data and mathematics with (theoretical) idealization. Act two reports the ease with which the computational approach incorporated quantum theory. The Lennard-Jones potential occupied a leading position. Act three welcomes the computer on the stage. Pioneering works in the 1950s and 1960s explored simulation methods to solve the "classical" equations for a large number of particles. Molecular dynamics grew into a widely used tool in both science and engineering for predicting the properties of materials. In this field, the LJ fluid acquired paradigmatic status ("the ubiquitous").

Act four offers a surprising twist. Recent work reports problems with reproducibility of LJ simulations. Although the simulations target the mathematically defined ideal object, the object that is actually simulated is different. This leads to the question of what the simulated LJ fluid actually is. Answering this "what" question requires an inquiry into the "how" question, i.e., into the methodology of simulation modeling. Viewed from the perspective of simulation, there is an under-examined layer of modeling steps that are relevant for many properties—and finally for the identity—of the simulated LJ fluid. Hence the allegedly most ideal of all fluids, created by mathematical prediction, turns out to have a bricolage character in practice.

Keywords: engineering thermodynamics, philosophy, history, simulation modeling

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