Classification of particle interaction potentials based on physical parameters of particle system

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In systems with different potential of particles interaction, physical quantities can differ [1]. The main factor of the interaction can be the gravitational potential, the Lennard-Jones potential, its modifications etc. Examples of such systems are different materials or the composition of different space systems such as gas stars. In this work, I investigated the sensitivity of the transfer coefficients and other physical quantities to a change in the interaction potential, both in the form of a change in the parameters of the potential, and in the form of a functional change. The question of the "proximity" of potentials in the sense of their influence on the macroparameters of systems is investigated. Calculations are carried out in the LAMMPS software package. On the basis of the studied characteristics of the systems, I made a classification of the potentials of different functional behavior. For classification is done by using machine learning methods with small databases, assuming a priori distribution. Current work shows that, despite the functional difference, different potentials can realize the same macroparameters in the system. It turns out that this phenomenon is observed in real life and corresponding examples are given. On the basis of the results obtained, the I discussed the question about what can be expected from structures that are (so far) guessed in computational physics but have not yet been obtained experimentally.

[1] Whipple E C 1981 *Rep. Prog. Phys* **4** 206–210