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Development of a Computer-Simulation Model for Particle Filling Based on Molecular Dynamics

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Abstract. This scientific work presents the development of a computer-simulation model for particle filling in three-dimensional space based on molecular dynamics methods. The Lennard-Jones potential was used to simulate interactions between particles, and the equations of motion were integrated using the Velocity Verlet algorithm. The model incorporates periodic boundary conditions (PBC), ensuring accurate representation of an infinite system without boundary effects. The simulation results confirm the system's energy stability: the total energy remains virtually unchanged throughout the simulation, indicating the correctness of numerical integration. Fluctuations in kinetic and potential energies demonstrate normal system dynamics, where energy is redistributed among particles through interactions. An analysis of the spatial distribution of particles revealed that the system remains in a liquid state, with no signs of solid structure formation or particle aggregation. Notably, the developed model enables the simulation of complex physical processes such as dense structure formation, particle transport, and self-packing. The obtained results highlight the efficiency of the molecular dynamics method for analyzing granular and particulate media, as well as for studying the physical properties of multi-particle systems. The model can be utilized to optimize technological processes related to material transportation, packaging, and storage, as well as for research into nanomaterials and composites.

1 Introduction

Molecular dynamics is one of the key methods of computer simulation that enables the study of the dynamic behavior of multi-particle systems at the atomic and molecular levels [1]. The use of the Lennard-Jones potential [2] to describe interparticle interactions and the Velocity Verlet integration algorithm [3] ensures accurate energy conservation and numerical stability of the system.

A crucial aspect of modelling is the analysis of the system's physical characteristics [4], such as particle distribution [5], their motion and interactions [6], and phase state [7]. Simulation studies to confirm the system's stability and validate the chosen modelling parameters – particularly the use of periodic boundary conditions (PBC) – allow the modelling of an infinite system while avoiding boundary effects and creating conditions closely approximating reality. The obtained results also enable the analysis of energy distributions (kinetic, potential, and total), the nature of particle motion, and possible structural formations in three-dimensional environments.

The conducted modelling allows understanding of how particles interact, form phase structures, or remain in liquid or gaseous phases. Thus, the development of a particle-filling computer application incorporating elements of molecular dynamics is a highly relevant task today. This research primarily aims to demonstrate the efficiency of applying molecular dynamics methods to