

MD Simulation of Argon and its solid-liquid transition

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ABSTRACT

I have simulated Argon using 864 particles for solid, liquid and gas phase. I have successfully computed the pressure and the pair-correlation function. I have computed the diffusion coefficient, but an error remains. I have parallelised the force calculation for a speed-up of 2.33 on 3 cores. Then I have studied the phase transition from solid to liquid and posed a hypothesis when this phase transition occurs. Future research is required to study the crystallization process (liquid to solid), for very small temperature steps are required.

Keywords

randomized algorithms, primality, SS, MR, AKS

1. INTRODUCTION

It is a tedious job to measure material properties of all materials, for there are infinitely many; Let the temperature-dependency for all of them, etc. Let us learn from e.g. engineers who had to predict whether a bridge design would collapse, or whether an ocean protection barrier would hold. Back in the days, they would build a scaled-down model and use that prototype to provide an answer. Nowadays, they are able to use the computer to simulate the situations in far less time and with far more accuracy than they were used to be able.

The power of the computer may be used in material sciences as well. We may, for example, compute the diffusion coefficient numerically, rather than measuring it.

Verlet (1967) [1] was one of the pioneers in this area. While his simulations had to run for days, our simulations may run for several minutes, allowing us to simulate far more details.

In my molecular dynamics simulation (MDS), I will redo some of Verlet's work to validate my simulation. The material under consideration is Argon. I will look at properties like the pair-correlation function, pressure, diffusion, parallelisation of the algorithm and phase-transitions.

2. THEORY

I have simulated Argon using 864 particles for solid, liquid and gas phase. I have successfully computed the pressure and the pair-correlation function. I have computed the diffusion coefficient, but an error remains. I have parallelised the force calculation for a speed-up of 2.33 on 3 cores. Then I have studied the phase transition from solid to liquid and posed a hypothesis when this phase transition occurs. Future research is required to study the crystallization process (liquid to solid), for very small temperature steps are required.

3. RESULTS

I have simulated Argon using 864 particles for solid, liquid and gas phase. I have successfully computed the pressure and the pair-correlation function. I have computed the diffusion coefficient, but an error remains. I have parallelised the force calculation for a speed-up of 2.33 on 3 cores. Then I have studied the phase transition from solid to liquid and posed a hypothesis when this phase transition occurs. Future research is required to study the crystallization process (liquid to solid), for very small temperature steps are required.

4. CONCLUSIONS

I have successfully simulated Argon in solid, liquid and gaseous form. I have computed the pressure, and shown that the computed pressure is in agreement with Verlet's original paper, but as well that the pressure matches nature at 0 °C. Pair-correlation functions have been created, which show clear differences between the three phases. I have attempted to compute the diffusion coefficient, and I have found the right order of magnitude. At the same time, the graphs show there is still a bug present, so further attention is needed to find more accurate predictions for the diffusion coefficient. I have qualitatively looked into the phase transition from solid to liquid and theorised that the phase transition occurs when particles oscillate sufficiently much such that they can 'touch' each other and thus cause a snow-ball effect, destroying the crystal lattice. Further research is required to study this phase transition and the other 3 phase transitions in more detail.

5. REFERENCES

- [1] L. Verlet. Computer 'experiments' on classical fluids: Thermodynamical properties of lennard-jones molecules. *Physical Review*, 159(1), July 1967.