Project 5 FYS4150

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Abstract

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1 Introduction

MD: "Numerical method for studying many-particle systems such as molecules, clusters, and even macroscopic systems such as gases, liquids and solids "

Kjetils notater: Simulere bevegelse N atomer og molekyler basert på klassisk newtonsk dynamikk: $F_i = m\frac{\mathrm{d}ri}{\mathrm{d}t} = -\frac{\partial U}{\partial r:i}$. Kraften er ofte sterkt avstandsavhengig og kan komme fra eks. Lennard Jones potensial. [1].

Fysikk:

Material science: Can use potentials dervied from non-relativistic Schrödinger equation to investigate lattic and defect dynamics at atomistic scale. [2]

Kjemi: behavoiur ideal gas, chemical reacton $A+A \rightarrow B+B$ with hard sphere potential and Lennard Jones potential, [3]

Bio: Simulate membranes

God link til "hva er MD": https://udel.edu/ arthij/MD.pdf

References

[1] Vincent E. Lamberti, Lloyd D. Fosdick, Elizabeth R. Jessup, and Carolyn J. C. Schauble. A hands-on introduction to molecular dynamics. *Journal of Chemical Education*, 79(5):601, 2002.

[2] Martin O Steinhauser and Stefan Hiermaier. A review of computational methods in materials science: Examples from shock-wave and polymer physics. *International Journal of Molecular Sciences*, 10(12):5135–5216, 12 2009.

[3] J. Gorecki and J. Gryko. Molecular dynamics simulation of a chemical reaction. *Computer Physics Communications*, 54(2):245 – 249, 1989.

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