Report for Computer Simulation of Physical Systems I
Autumn semester 2025-2026

General information
This report explores the physical properties of a Lennard-Jones liquid, calculated using various simulation techniques presented in the course. These techniques include NVE molecular dynamics, Nosé-Hoover molecular dynamics, and Monte Carlo simulations.

Deadline and submission method
The report is due on **Wednesday, 17 December 2025, by 13:00**. It must be submitted through both

i. uploading on Moodle page, and
ii. handing-in of paper version (office PH^{H2}467 or green mailbox in front of office).

Instructions
All simulations concern liquid argon with Lennard-Jones parameters ε/k_B = 120 K and σ = 3.4 Å as in the paper of Rahman [1]. Further, all simulations should be performed primarily at T = 94,4 K, ρ = 1.374 g/cm^{-3}, using N = 864 particles, and using a timestep of Δt = 0.01 ps following Rahman [1]. The influence of these simulation parameters can be addressed in the discussions.

For each physical quantity listed in the table below, follow these steps:

1. **Data collection**
    - Use the specified methods to obtain the physical quantity.
    - Utilize the provided codes from the exercise sessions to gather your results.
2. **Data presentation**
    - Present your results using one or more graphs containing labels with units along the axes.
    - Express physical quantities in physical units, not in Lennard-Jones units.
    - Define all quantities presented in the graphs in the figure captions.
3. **Discussion of results**
    - Discuss your findings, referring to the guidelines given in the table for each physical quantity.

Format
- **Length**: max 7 A4 pages (including references) + cover page.
- **Margins**: 2 cm.
- **Font**: 12 pt Helvetica or (New) Times-Roman. Helvetica or (New) Times-Roman or the PYTHON default font “DejaVu Sans” are accepted for the figures.
- **Line spacing**: 1.25.
- **Number of columns**: one column.

Contents of the report

Physical quantity	Task	
Pair correlation function $g(r)$	Calculate $g(r)$ through NVE molecular dynamics. Produce a histogram plot in real space.	
	Calculate $g(r)$ through Nosé-Hoover molecular dynamics. Produce a histogram plot in real space.	
	Calculate $g(r)$ through Monte Carlo simulation. Produce a histogram plot in real space.	
	Discussion: comparison with results from Ref. [1]; comparison of results obtained with molecular dynamics and Monte-Carlo.	
Structure factor $S(k)$	Calculate $S(k)$ through Fourier transformation of $g(r)$ obtained through NVE molecular dynamics	
	Calculate $S(k)$ through direct sampling method using the NVE molecular dynamics	
	Discussion: comparison with results from Ref. [1]; comparison of results obtained with Fourier transform and with direct method.	
Diffusion coefficient D	Calculate D from the dependence of the mean square displacement on time (Einstein's formula) using the NVE molecular dynamics.	
	Calculate D from the velocity-velocity autocorrelation function using the NVE molecular dynamics.	
	Discussion: comparison with results from Ref. [1]; determine the statistical errors and discuss advantages and limitations of the two methods.	
Average potential energy U	Calculate the average potential energy U using the Monte Carlo method.	
	Determine the error ΔU on the average potential energy U using the blocking analysis.	
	Discussion: examine what information on the time correlation can be extracted from the blocking analysis.	

[1] A. Rahman, *Correlations in the Motion of Atoms in Liquid Argon*, Phys. Rev. **136 A**, 404 (1964).