Aalto University
School of Science

PHYS-E0412 Computational Physics, exam 27.8.2018

1. Monte Carlo integration, importance sampling and the Metropolis algorithm (8p)

   Explain the basic principles of Monte Carlo integration and related error estimation. What are the main benefits of this method? What does importance sampling mean and why is it used? Describe the purpose and the main idea of the so-called Metropolis algorithm.

2. Phases of matter with molecular dynamics (5p)

   Describe in detail how you would study the phases of matter at finite temperatures using molecular dynamics and a given pair potential? How do you set up a model system? How would you propagate it in time and measure physical quantities? Provide some examples of quantities you can use to quantify the phases you observe in the simulation.

3. Solution of the Poisson equation (8p)

   In a general domain Ω the Poisson equation

   $$\begin{cases} -\Delta u = f \text{ in } \Omega \\ u = 0 \text{ on } \partial\Omega \end{cases}$$

   needs to be solved using numerical methods. Describe steps required to obtain the solution when Ω is a two-dimensional domain. Consider all stages required to obtain the approximate solution u_h and discuss briefly their merits and limitations.

4. The heat and the wave equation (5p)

   The time-dependent problems, the heat equation $\partial_t u = \Delta u$ and the wave equation $\partial_{tt} u = \Delta u$ require computational methods that are different from those used for the time-independent Poisson problem. Describe time-integration methods suitable for such time-dependent problems and discuss their merits and limitations. (5 p.)