Simulations in Many-particle Physics TMF021 – exam questions 2021/2

1. Integration by MC method - simple and preferential sampling, central limit theorem and error of MC method, comparison with standard numerical integration. Generation of pseudorandom numbers with general distribution.
2. Stochastic processes, transition matrix, Markov chains, detailed balance, microscopic reversibility, existence of limiting distribution.
3. Implementation of Monte Carlo step for canonical distribution (generation and acceptance of test configuration). Metropolis and Barker method.
4. Application of MC to geometric problems: random walks, percolation (threshold calculation, Hoshen-Kopelman algorithm), diffusion-limited aggregation.
5. Thermodynamic MC - demonstration on Ising model, calculation of specific heat and susceptibility, determination of critical temperature.
6. Cellular automata (CA) - types and definitions of CA, dependence of the number of CA on dimension, examples of CA: one-dimensional CA, game of life, lattice gas, sand pile.
7. Verlet and Gear MD integrators, choice of integrator and integration step.
8. Radial distribution function, expression for the mean value of a quantity (e.g. energy) using the integral of a pair function (e.g. potential) and RDF, long range correction to energy.
9. Temperature in MD, thermostats (velocity rescaling, Berendsen frictional, Andersen).
10. Pressure measurements in MD/MC, MD simulations at constant pressure; NPT ensemble in MC.
11. Molecular potentials (intermolecular and intramolecular), combining rules.
12. Technical details of MC - algorithm for calculation of energy change, trial displacement generation, acceptance ratio, range of potential vs. system size, boundary conditions.
13. Non-Boltzmann sampling of configurational space, methods for efficient sampling of configurational space (principles of metadynamics, potential of mean force, parallel tempering).