Computational Physics

Topics for the Complex Exam

1. Internal number representation of digital computers, rounding and truncation errors. Numerical differentiation using finite differences. Classical methods of numerical integration (trapezoidal rule, Simpson's rule, Romberg integration, Gauss quadrature).
2. Numerical solutions of nonlinear equations and systems of equations. Optimization methods (Newton's method, conjugate gradient method, simulated annealing).
3. Fourier transform: DFT, FFT; and basic applications in physics (correlation, convolution, filtering, etc.).
4. Numerical methods for initial value problems of ordinary differential equations (Runge–Kutta with step-size control, predictor–corrector methods, backward differencing methods).
5. Boundary value problems of ordinary differential equations. Numerical solution of the one-dimensional time-independent Schrödinger equation using the Numerov method.
6. Molecular dynamics simulations (numerical integration of classical MD equations of motion, modeling canonical and isobaric-isothermal ensembles — NVT and NPT).
7. Basics of Monte Carlo methods and their key applications in (statistical) physics (sampling, Markov chains, ergodicity).
8. Numerical solution of wave propagation problems (typical initial value problems and boundary conditions; Lax method, von Neumann stability analysis, numerical dissipation and dispersion, second-order methods).
9. Numerical solution of diffusion problems (typical initial value problems and boundary conditions; Crank–Nicholson method, unitary discretization of the time-dependent Schrödinger equation, operator splitting method).
10. Numerical solution of the Poisson equation (typical boundary conditions; finite difference methods: direct matrix methods, Fourier method, relaxation method, operator splitting; basics of multigrid and finite element methods).
11. Capabilities of symbolic mathematics software (e.g., Mathematica, Maple) relevant to physical applications (differentiation, integration, optimization, equation solving, differential equations, etc.).

Recommended Literature

1. W. H. Press, S. A. Teukolsky, W. T. Vetterling, B. P. Flannery: *Numerical Recipes in C*, Cambridge University Press, 2nd ed., 1992
2. I. N. Bronstein, K. A. Semendjajev, G. Musiol, H. Mühling: *Handbook of Mathematics*, Typotex Publishing, Budapest, 2002
3. Michael T. Heath: *Scientific Computing: An Introductory Survey*, McGraw-Hill, New York, 2002
4. Bogár et al.: *Computational Biochemistry*, 2013, Chapters 2 and 6 (http://eta.bibl.u-szeged.hu/1297/1/ computational_biochemistry.pdf)