Physics 5403: Computational Physics

Instructor: Thomas Vojta
The course has a lecture and a lab component.

Contents of the lectures

1. **Introduction**
   - 1.1 What is computational physics?
   - 1.2 Languages and algorithms
   - 1.3 Good practise in computational physics
   - 1.4 Plan of the course
2. **Basic numerical methods**
   - 2.1 Interpolations and approximations
   - 2.2 Differentiation and integration
   - 2.3 Zeros and extremes of a single-variable function
   - 2.4 Random numbers
3. **Ordinary differential equations**
   - 3.1 Initial value problems
   - 3.2 Application: Chaotic dynamics of a driven pendulum
   - 3.3 Boundary value problems
   - 3.4 Eigenvalue problems
   - 3.5 Application: One-dimensional Schrödinger equation
4. **Numerical methods for matrices**
   - 4.1 Matrices in physics
   - 4.2 Scientific software libraries
   - 4.3 Linear equation systems
   - 4.4 Application: Zeros and extremes of a multi-variable function
   - 4.5 Matrix eigenvalue problems
5. **Spectral analysis**
   - 5.1 Fourier transformation and orthogonal functions
   - 5.2 Discrete Fourier transformation and Nyquist theorem
   - 5.3 Fast Fourier transformation
   - 5.4 Application: Autocorrelation function and power spectrum of a driven pendulum
   - 5.5 Fourier transformation in higher dimension
   - 5.6 Application: Scattering cross section and structure factor

5.7 Wavelet analysis

6. **Molecular dynamics simulations**

   6.1 Basic machinery

   6.2 Time integration – Verlet algorithm

   6.3 Geometry and boundary conditions

   6.4 Running, measuring, analyzing

   6.5 Molecular dynamics as an optimization tool

7. **Monte-Carlo simulations**

   7.1 Sampling and integration

   7.2 Random walks, self-avoiding walks, and diffusion

   7.3 Percolation and cluster growths

   7.4 Metropolis algorithm

   7.5 The Ising model in statistical physics

   7.6 Phase transitions and critical behavior

Example Lab Projects (Actual assignments will be posted on the course web page.)

- Warmup and error analysis
- Simulation of radioactive decay
- Diffusion and random walks
- The solar system
- Chaos in the driven damped pendulum
- Quantum eigenstates in a potential well
- Geometric structure of multi charge clusters
- Power spectrum of a driven damped pendulum
- Structure and diffraction patterns of crystals and quasicrystals
- Molecular dynamics simulation of a Lennard-Jones gas
- Percolation and cluster growth
- Critical phenomena in an Ising model