Chapter 1

Introduction

1.1 General

For **physics students** the computational quantum physics courses is a recommended prerequisite for any computationally oriented semester thesis, proseminar, master thesis or doctoral thesis.

For **computational science and engineering (RW) students** the computational quantum physics courses is part of the "Vertiefung" in theoretical physics.

1.1.1 Exercises

Programming Languages

Except when a specific programming language or tool is explicitly requested you are free to choose any programming language you like. Solutions will often be given either as C++ programs or Mathematica Notebooks.

Computer Access

The lecture rooms offer both Linux workstations, for which accounts can be requested with the computer support group of the physics department in the HPT building, as well as connections for your notebook computers.

1.1.2 Prerequisites

As a prerequisite for this course we expect knowledge of the following topics. Please contact us if you have any doubts or questions.

Computing

- Basic knowledge of UNIX
- At least one procedural programming language such as C, C++, Pascal, Java or FORTRAN. C++ knowledge is preferred.
- Knowledge of a symbolic mathematics program such as Mathematica or Maple.
- Ability to produce graphical plots.

Numerical Analysis

- Numerical integration and differentiation
- Linear solvers and eigensolvers
- Root solvers and optimization
- Statistical analysis

Quantum Mechanics

Basic knowledge of quantum mechanics, at the level of the quantum mechanics taught to computational scientists, should be sufficient to follow the course. If you feel lost at any point, please ask the lecturer to explain whatever you do not understand. We want you to be able to follow this course without taking an advanced quantum mechanics class.

1.1.3 References

1. J.M. Thijssen, *Computational Physics*, Cambridge University Press (1999) ISBN 0521575885
2. Nicholas J. Giordano, *Computational Physics*, Pearson Education (1996) ISBN 0133677230.
3. Harvey Gould and Jan Tobochnik, *An Introduction to Computer Simulation Methods*, 2nd edition, Addison Wesley (1996), ISBN 00201506041
4. Tao Pang, *An Introduction to Computational Physics*, Cambridge University Press (1997) ISBN 0521485924

1.2 Overview

In this class we will learn how to simulate quantum systems, starting from the simple one-dimensional Schrödinger equation to simulations of interacting quantum many body problems in condensed matter physics and in quantum field theories. In particular we will study

- The one-body Schrödinger equation and its numerical solution
- The many-body Schrödinger equation and second quantization
- Approximate solutions to the many body Schrödinger equation
- Path integrals and quantum Monte Carlo simulations
- Numerically exact solutions to (some) many body quantum problems
- Some simple quantum field theories