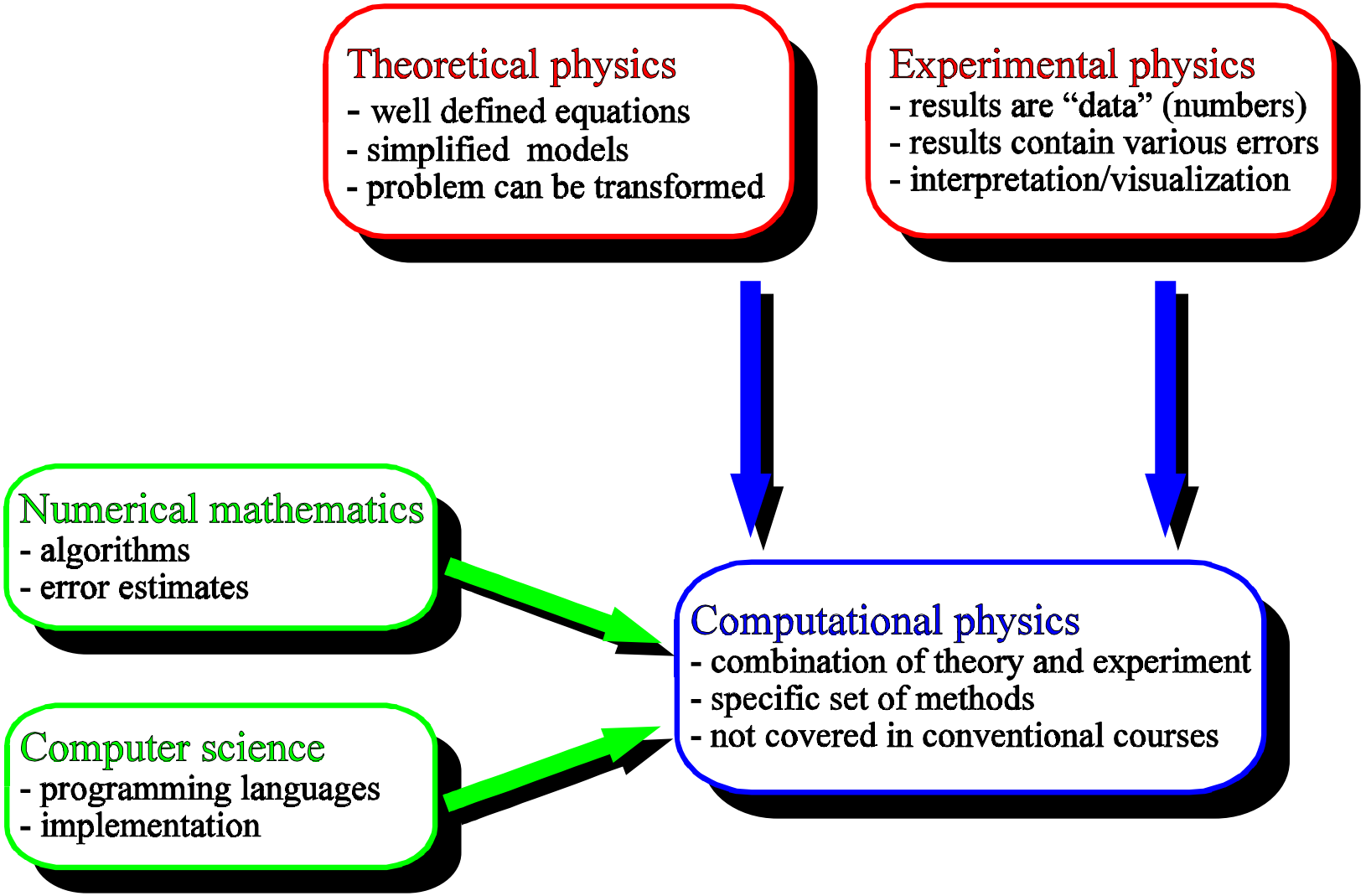
Condensed Matter Physics on the Computer - A Laboratory Style Graduate Course

Michael Schreiber and Thomas Vojta

Institut für Physik, Technische Universität Chemnitz,
D-09107 Chemnitz, Germany

1. **Teaching Computational Physics**
2. **Design of the course**
3. **Physics and computational topics**
4. **Example problems**


Theoretical physics
- well defined equations
- simplified models
- problem can be transformed
Experimental physics
- results are "data" (numbers)
- results contain various errors
- interpretation/visualization
Numerical mathematics
- algorithms
- error estimates
Computer science
- programming languages
- implementation
Computational physics
- combination of theory and experiment
- specific set of methods
- not covered in conventional courses

Teaching computational physics: What do we want to achieve?

Teach students to **solve a physical problem** using a computer simulation

This includes:

- analyzing the physical problem
- reformulating the problem in a way suitable for a simulation
- choosing an efficient numerical algorithm
- writing the computer code
- running the computer simulation
- analyzing and interpreting the data obtained

A laboratory style computational condensed matter physics course

- taught several times at the universities of Dortmund, Mainz and Chemnitz
- aimed at beginning graduate students (3rd and 4th year students in Germany)

Structure of the course:

- consists of separate condensed matter physics problems to be solved using computer simulations
- each course unit comprises a lecture (one hour) and tutored computer work (two hours)
- the lecture covers basic physical ideas and algorithmical aspects
- computer work: students develop programs, run simulations and analyze and visualize the data

What it is not ...

Course concentrates on **computational physics** aspects

It is therefore

- not a replacement for a conventional course in condensed matter physics; instead, it is best taught in parallel to or right after such a course
- not a course in numerical mathematics; algorithmical questions are discussed only to the extend necessary to solve the problem; usually a rather simple method is used
- not a programming course; some programming experience is expected, most students have already used a programming language at this stage

Implementational details:

- students develop programs from scratch
- no code is provided except for very few subroutines, e.g. for eigenvalue problems
- FORTRAN 90/95 is the language supported in the course
- students are allowed to use a different programming language (usually C, C++ or Pascal)
- visualization of the results via GNUPlot

Summary of topics

Algorithmic preliminaries

- series expansions (power series, Fourier series)
- random numbers (generation, distributions)

Random walks and growth models

- polymer statistics (simple walks and self-avoiding walks)
- percolation, diffusion limited aggregation (self-similarity, fractals)

Phonons

- dispersion of linear chain and square lattice
- phonon focusing
- molecular dynamics simulations

Electronic states

- band structure (dispersion relation, density of states)
- electronic hopping transport (nearest neighbor and variable range hopping)
- Anderson localization (localization length, metal-insulator transition)

Thermodynamics and related problems

- Ising model (equilibrium properties, phase transition)
- cellular automata for chemical reactions
- simulated annealing, traveling salesman

Summary of computational techniques

- integration of ordinary differential equations (e.g., Newtons equations)
- eigenvalue problems (e.g. stationary Schrödinger equation)
- transfer matrix methods
- Stochastic methods:
  - random walks (simple sampling Monte Carlo)
  - Metropolis algorithm (importance sampling Monte Carlo)
  - dynamical Monte Carlo
  - stochastic optimization

Conclusions

- computational physics combines a unique set of techniques from theoretical physics, experimental physics, numerical mathematics, and computer science

- teaching computational physics, i.e. teaching how to solve a physics problem using computer simulations, therefore requires specific types of courses

- we have successfully used a laboratory style course to teach computational condensed matter physics

- **course consists of a set of separate physics problems the students solve by**
  - analyzing the physical problem
  - reformulating the problem in a way suitable for a simulation
  - choosing an efficient numerical algorithm
  - writing the computer code (from scratch)
  - running the computer simulation
  - analyzing and interpreting the data obtained

- **selection of problems is made to**
  - cover a wide variety of computational techniques
  - provide connections to state-of-the-art research topics

Condensed Matter Physics on the Computer - Example problems

Michael Schreiber and Thomas Vojta

Institut für Physik, Technische Universität Chemnitz,
D-09107 Chemnitz, Germany

1. Hopping conductivity in semiconductors
2. Damage spreading in kinetic Ising models

3. Anderson localization of disordered electrons

Hopping conductivity and damage spreading:

extensions and generalizations of basic equilibrium Monte Carlo (Metropolis) algorithms as taught in the Ising model problem

Hopping conductivity: dynamics close to equilibrium
Damage spreading: dynamics far from equilibrium

Anderson localization of disordered electrons:

transfer matrix methods, finite size scaling ☞ M. Schreiber (Saturday)

Example: Hopping conductivity in semiconductors

Prerequisites: Problems on random numbers and on the Monte Carlo simulation of the Ising model

Goal: Investigation of the electrical transport in weakly doped semiconductors at low temperatures

Physics background:

- at low temperatures weakly doped semiconductors are insulators
- electrons can move by thermally (phonon) assisted hopping between localized impurity states
- without external electric field electrons can hop in all directions with equal probability ☞ no resulting current
- with electric field hopping probability depends on field ☞ net current results

Specific tasks:

- determine dependence of current on external voltage
- calculate conductivity
- study its temperature dependence

A simple model for the hopping transport problem

- linear, square or cubic lattice of (impurity) sites i with one electron state per site
- potential φ_i at site i is random, drawn from an interval $[-W, W]$, to model the random environment of an impurity
- hopping is possible downwards in energy by emission of a photon or upwards in energy by absorption of a photon
- hopping rate W_{ij} between two sites depends on distance $r_{ij}=|\mathbf{r}_j-\mathbf{r}_i|$ and on potential difference $\Delta V_{ij} = \varphi_j - \varphi_i - \mathbf{E}\cdot(\mathbf{r}_j-\mathbf{r}_i)$ ($\mathbf{E}$ is the external electric field)

$$W_{ij}=\begin{cases} \exp(-r_{ij}/2a) & \Delta V_{ij}<0 \\ \exp(-r_{ij}/2a-\Delta V_{ij}/T) & \Delta V_{ij}>0 \end{cases}$$

(a = localization length of impurity state, T = temperature)

- hopping process with these rates can be simulated by Monte Carlo procedure

Schedule for the computer work

First day:

- develop a Monte-Carlo program for thermally assisted hopping in a one-dimensional impurity band
- study diffusion of electrons without external electric field

Second day:

- determine the dependence of the current on the electric field, check Ohm's law, calculate the conductivity
- determine the temperature dependence of the conductivity
- discuss the various regimes (nearest neighbor hopping and variable range hopping

Optional:

- try other approaches to calculate conductivity (Kubo formula)

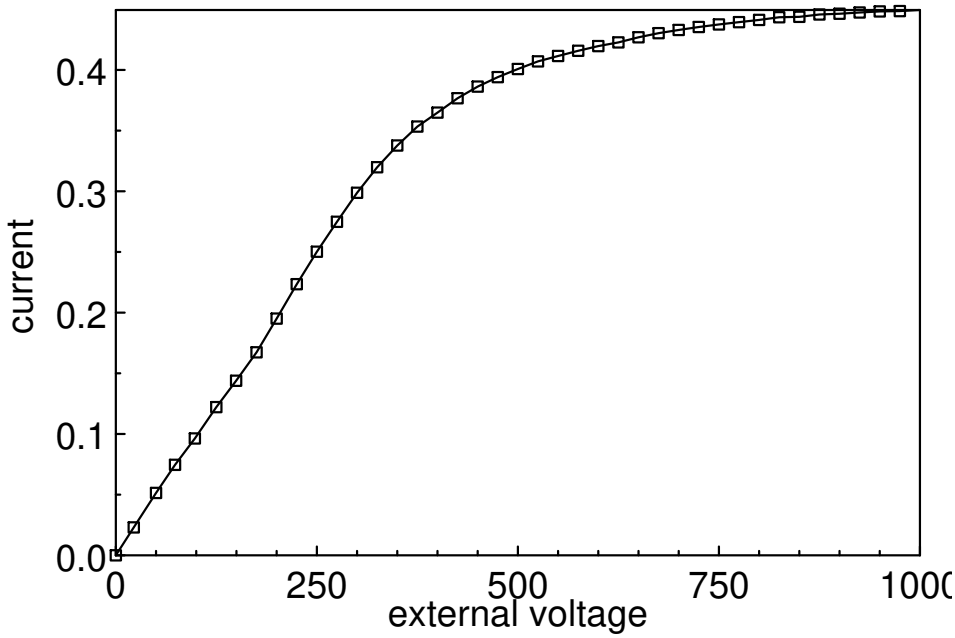
Connection to state-of-the-art research

Course problem: hopping transport of **non-interacting** electrons
well understood in general

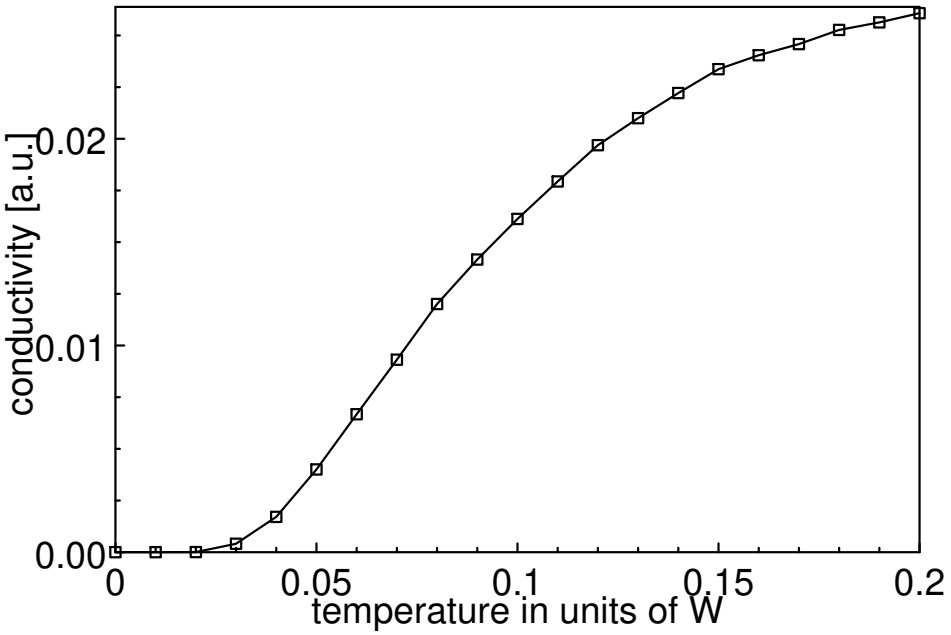
However: real electrons **interact** via Coulomb potential
hopping transport of interacting electrons not fully understood today

Questions: What are the hopping entities, single electrons, pairs, clusters?
How do they couple to the phonons?
What is the temperature dependence of the resulting conductivity?

Results



Current voltage characteristics for a chain of 1000 sites, W=1, T=0.2, a=2.



Temperature dependence of the conductivity.