Computational Physics

Introduction and fundamentals

Overview of the course

week	topic
1	Introduction and fundamentals
2	Fully discrete problems
	Ordinary differential equations
3	Introduction, error & convergence
4	Stability and operator exponential
	Partial differential equations
5	Mass-spring problems and PDEs
6	Finite difference time domain
7	Stability and frequency domain
8	Spectral discretizations
9	Variational forms of frequency-domain problems
10	Finite elements
11	Green function based methods I
12	Recap and Q&A

Format

The course is taught in the following format:

- 1.5-2 hours discussion of exercises at begin of lecture slot
- 1.5-2 hours lecture afterwards
- Weekly problem sheet with exercises (analytics and programming e.g. in matlab)
- Ideally do the problem in groups
- The problems are the main teaching instrument

Why computational physics?

- Physics is the attempt to construct a quantative mathematical model of the universe.
- The model takes the form of equations
- They must be "occasionally" evaluated
  a. to test it against experiments
  b. to use it for engineering
- Few problems have an exact analytical solution
- The solutions of most problems can be approximated using some sort of expansion ansatz
- Doing this by hand to any reasonable accuracy is tedious, the opposite of creative and prone to random mistakes
- Perfect job for a computer

The suitable methods depend on the type of equation to be solved and the question. There are dozens of methods, depending on the problem.

Relation to experiments and analytic theory

Experiment:

- By definition covers entire physics (eliminating dirt effects challenging) and any realisable setting
- Probes individual points in parameter space
- Measurement inaccuracies
- Always quantitative results
- Expensive material, time consuming

Analytics:

- Idealized physics (including dirt effects challenging) and setting ("spherical cow in vacuum")
- Overview over entire parameter space
- Exact
- Quantitative results need numerics
- Very time consuming

Numerics:

- Idealized physics, but flexible setting
- Points in parameter space
- Numerical errors
- Quantitative
- Cheap and fast

From analytics to numerics

Quantative theory *always* works like this:

1. Question to be answered
   (e.g. “Will my bridge collapse during a storm?”)
2. Fundamental equations describing the basic physical model
   (e.g. Christoffel equation for continuum mechanics and Navier-Stokes equations for air flow)
3. Assumptions and analytical simplifications
   (e.g. 1. resonances excited by wind through nonlinearities; 2. equation for resonant states; 3. equation for nonlinear coupling)
4. Potentially further analytical steps to reduce the complexity of the subproblems
5. Numerical evaluation of simplified equations

- Every quantative theory requires numerics
- Every computation requires some degree of analytical calculation
- Rule of thumb: more analytical groundwork
  $\Rightarrow$ more specialized but also more efficient computations

Classification of physical problems

In this course we discuss methods for fairly general classical problems that can be classified as:

	transient	stationary
few particles or modes	ODE in time	fully discrete
continuous fields	PDE in space & time	PDE in space

Problems within each class are solved in a similar way, even though the physics might be very different.

There are many further classes, which we ignore, e.g.:

- Path integral methods
- Stochastic methods

They are typically very powerful but often quite specialized.

Some examples for these problem classes

1. ODE in time (weeks 3–5)
   - Time-evolution in mass-spring problems or celestial mechanics
   - Time-evolution in electronic circuit with lumped elements
   - Full Schrödinger equation with discrete operators (spins, angular momentum, atomic & molecular states)
2. fully discrete (week 2)
   - Equilibrium states, AC-response, transfer functions, energy-eigenstates and resonant frequencies of type-1 problems
3. PDE in space & time (weeks 6–8)
   - Transient diffusion e.g. of gases, of carriers in semiconductors, of heat in solids, of neutrons in nuclear reactor
   - Time-evolution of wave propagation (free space, waveguides or resonators) in electromagnetics and acoustics
4. PDE in space (weeks 9–12)
   - Stationary flow in aerodynamics, acoustic resonance
   - Electromagnetic resonators, electrostatics, magnetostatics
   - Static and dynamic stability in structural mechanics
   - Energy-eigenstates with quantum-mechanical wavefunctions

Aim of the course

The aim of the course is to

- Introduce some of the most common types of computational problems in classical physics and engineering
- Present some common strategies to solve them
- Highlight the problem of numerical error in its various forms

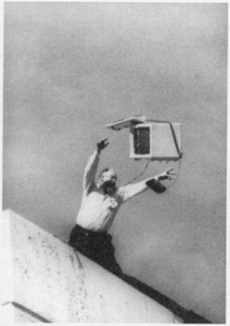

Photo Courtesy Al Neves.

Figure 12.1. I hurled this computer to its doom from atop National's 3-story parking garage. As the dust settled, I knew *that* computer would never lie to me again!

Bob Pease "Troubleshooting analog circuits", page 145

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Mathematical fundamentals: linear algebra

You should be comfortable with matrix algebra:

- Basic operations (addition, multiplication, inversion) of matrices and column-vectors
- Linear problems of the type $Ax = b$
- Eigenvalue problems of the type $Ax = \lambda x$
- Concept of bases and expansions

You should be familiar with basic linear algebra involving functions:

- Fourier transformation
- Taylor expansion
- Inner product and norms for functions: $\langle f, g \rangle = \int f^*(x) g(x) \mathrm{d}x$.

Mathematical fundamentals: calculus

You should be familiar with calculus and ODEs:

- Differentiation of chains, products, quotients and the usual fundamental functions (e.g. sin, sinh, exp, log)
- Integration using the usual tricks (mostly substitution & partial integration); also Dirac distribution $\delta(x)$
- How to analytically solve an arbitrary linear ODE with constant coefficients via Fourier transformation and by reduction to a first order system
- The concept of a Green function (a.k.a. fundamental solution, a.k.a. impulse response)

You should know about partial differential equations:

- Continuity equation $\partial_t \rho + \nabla \cdot j = 0$
- The Poisson equation $\Delta u(x, y) = s(x, y)$
- The 1d wave equation $\partial_t^2 u(x, t) + c^2 \partial_x^2 u(x, t) = 0$

Physical fundamentals

The examples in the exercises will be from these areas:

- Basic optics (mostly refraction at interface)
- Harmonic oscillator (classical and QM)
- Kepler problem (planetary orbit)
- Basic fluid dynamics
- 1d propagation of electromagnetic or water waves
- 2d acoustics (vibrations of a plate)
- Magnetostatics (field of a point dipole)

Homework

Make sure you have the fundamentals and read up if necessary.