Computational Physics I

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Certificates: “Sitzschein”, ECTS 6 credit points (oral exam),
“Studienbegl. Prüfung”, Diplomprüfung (2nd course required)

Change of time proposed: discuss (room availability to be checked)

Course Material

The lectures will introduce the methods and techniques for solving **physics problems** on the computer. Physics problems will be formulated and turned into algorithms which can be programmed. The general techniques for solving the differential equations, integrals, root finding, etc. which are encountered on the way will be presented. The errors which arise from digitization of real numbers, from approximations made in producing computer algorithms, and from input conditions will be analyzed.

The list of topics includes:

- error analysis
- polynommial interpolation
- Fourier transforms
- numerical derivatives
- ordinary and partial differential equations
- numerical integration
- solving systems of linear equations
- nonlinear equations, roots and extrema
- matrix diagonalization

Course Material

The idea is for the students to try out the algorithms themselves on their own computers. This is the best way to learn.

The recitation (exercise) sessions will be available for students who would like help in programming algorithms or visualizing results.

Recitation is from 14:15 - 15:45 in PH 1162 (CIP room)

An example

Simulation of the motion of a charged particle in a gas volume in a region with crossed electric and magnetic fields

$$\vec{F} = q(\vec{E} + \vec{v} \times \vec{B}) - \frac{dT}{ds}\widehat{v}$$

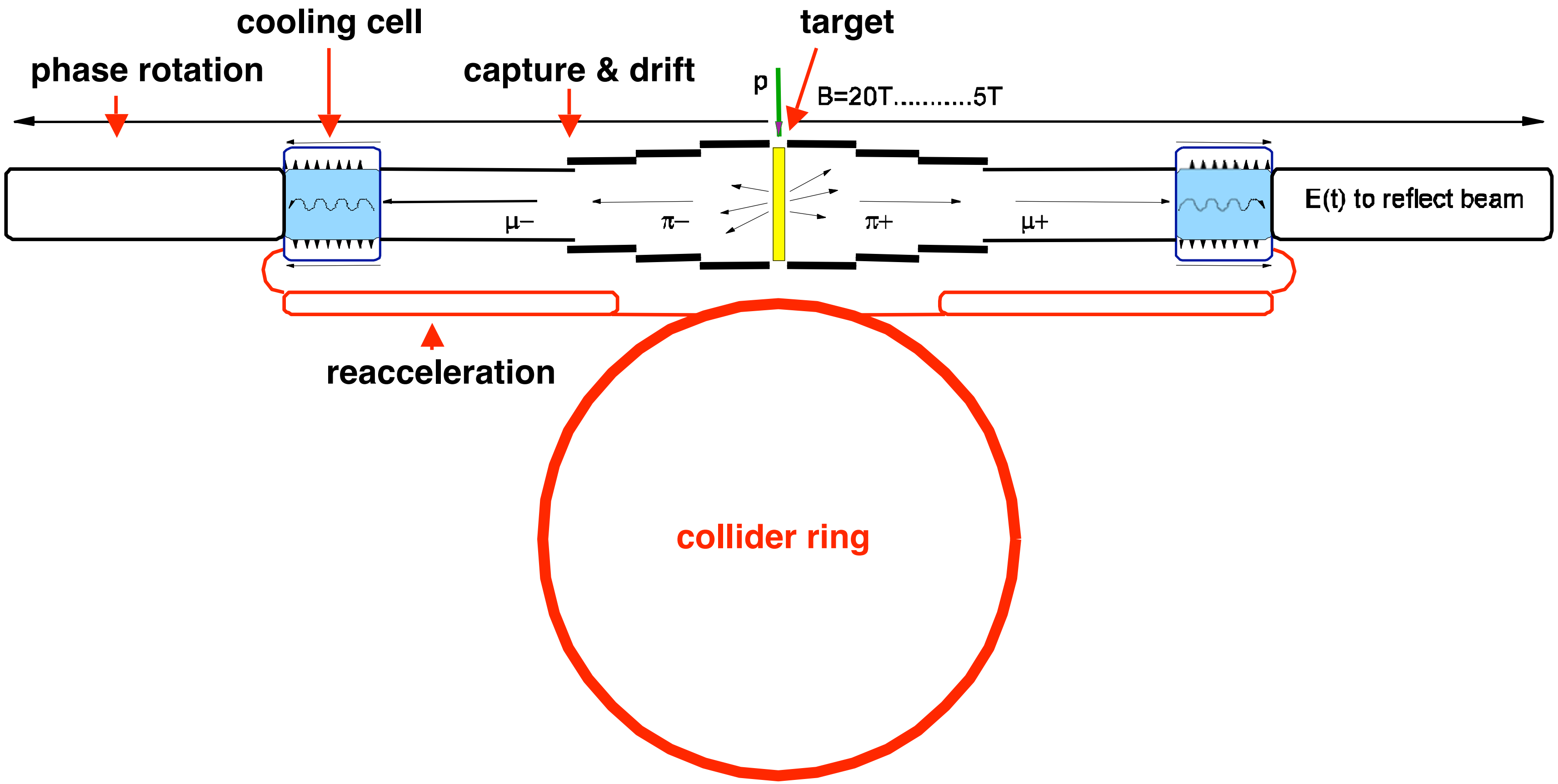
Force from Electric Field

Energy loss in gas

Force from magnetic field

Particle spirals around magnetic field line, slows down due to energy loss in gas and eventually moves at constant (Lorentz) angle.

Frictional Cooling



Simulating Derivatives

Doing it right is not obvious. E.g., look at simple oscillator:

$$\frac{d^2 x}{dt^2} = -\frac{k}{m} x$$

For numerical simulations, derivatives are replaced by differences. E.g.,

$$\frac{dv}{dt} = -\frac{k}{m} x \qquad \frac{dx}{dt} = v$$

$$v_{i+1} = v_i - \frac{k}{m} x_i \Delta t \quad x_{i+1} = x_i + v_i \Delta t$$

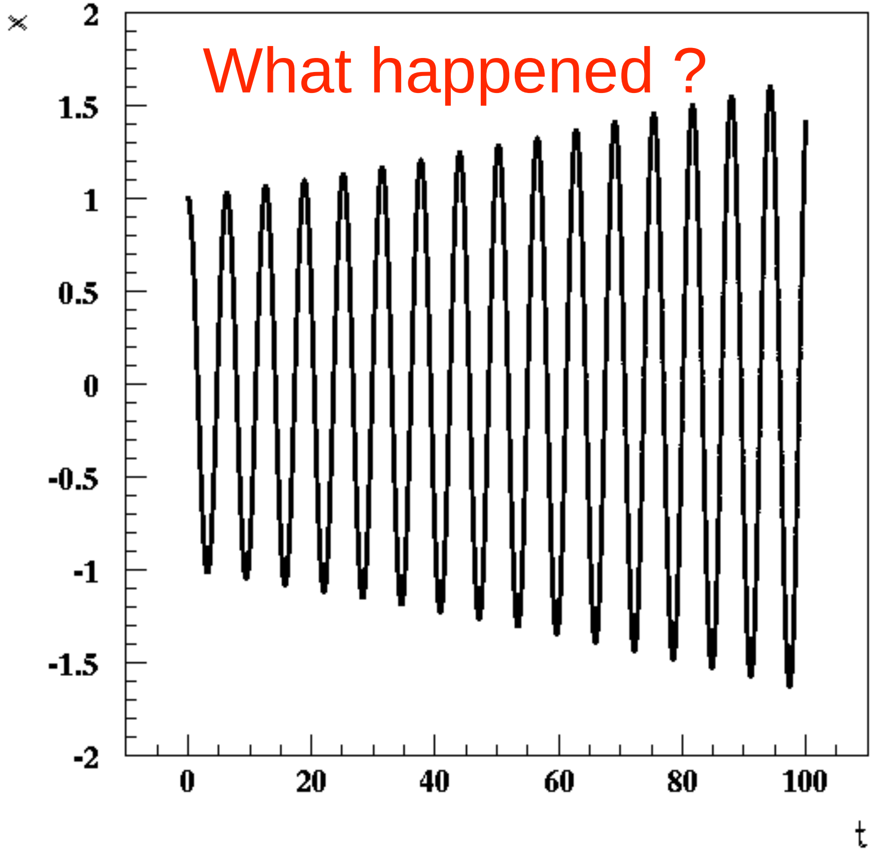
Euler algorithm

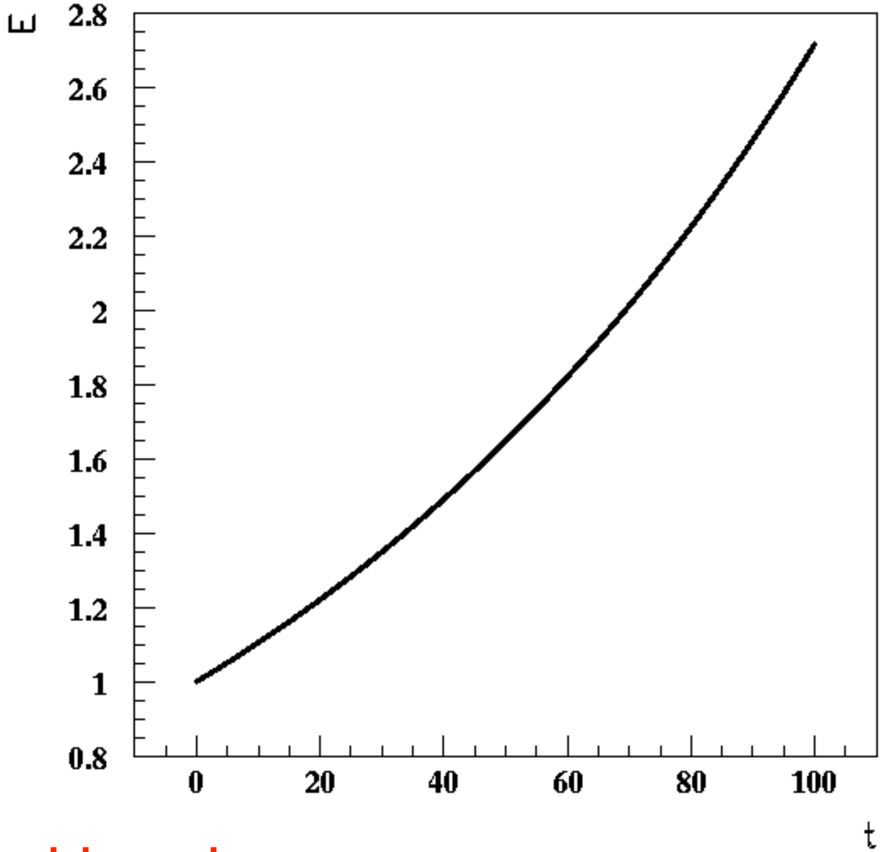
Need to specify initial conditions:

e.g., $x_0 = 1 \quad v_0 = 0$ Let's also take $\frac{k}{m} = 1$

Simple Oscillator

Choose a time step of 0.01, and here's what we get:





Algorithm does not conserve energy !

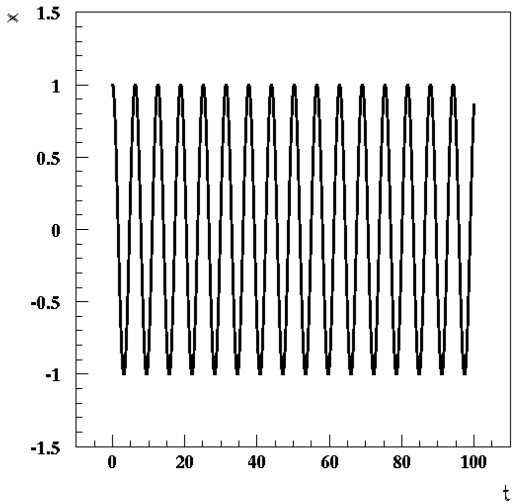
Simulating Derivatives

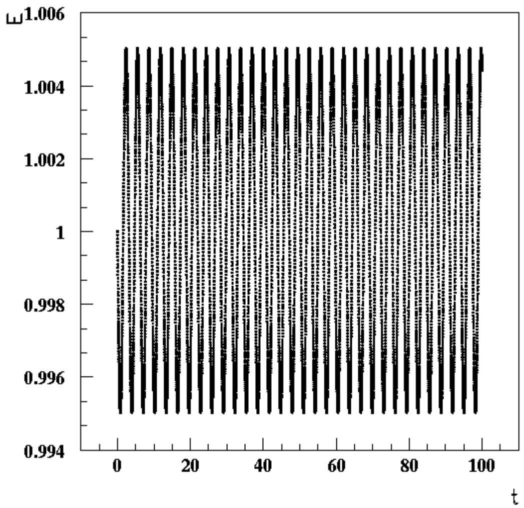
Now we make the simple change

$$\frac{dv}{dt} = -\frac{k}{m}x \qquad \frac{dx}{dt} = v$$

$$v_{i+1} = v_i - \frac{k}{m}x_i\Delta t \qquad x_{i+1} = x_i + \boxed{v_{i+1}}\Delta t$$

Euler-Cromer





Discovered by accident !

Message: need to show numerical algorithms adequate

Types of Uncertainties

We have just seen that algorithms can lead to incorrect results. Other sources of error are:

• Error in the input data (e.g., the initial conditions which we specified in the last problem). We will see how these uncertainties propagate to uncertainties in the final result. In non-linear systems, small changes in the input data can lead to huge changes at some later point $\Rightarrow$ chaos. (Example - driven pendulum).

$$\frac{d^2\theta}{dt^2} = -\frac{g}{d}\sin(\theta) - q\frac{d\theta}{dt} + F\sin(\Omega_D t)$$

Driving force

Gravitational force

Frictional force

Real number representation

• Numerical limitations of the computer. The computer works with integers in base 2. Real numbers are defined by a certain ‘bit’ pattern. A fixed number of bits is used, so that a largest and a smallest number are possible.

Computer language:	bit 1 or 0	$2^1=2$ possibilities
	byte - string of 8 bits,	$2^8=256$ possibilities
	word - 2 bytes	$2^{16}=65536$ possibilities
	longword - 4 bytes	$2^{32}=4{,}294{,}967{,}296$

Real numbers are usually represented by a bit combination.
‘Single precision’ $\equiv$ 4 bytes used to represent real number
‘Double precision’ $\equiv$ 8 bytes used to represent real number

Next time - go into detail into how numbers are represented on the computer.

Exercise Set 1

1. Reproduce the plots on p 7,8 of this lecture