introduction to computational physics

basic concepts and approaches

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experimantal physics IV - university of augsburg

outline

- motivation

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- motivation
- history of computing hardware/software

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- warning

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- computational techniques

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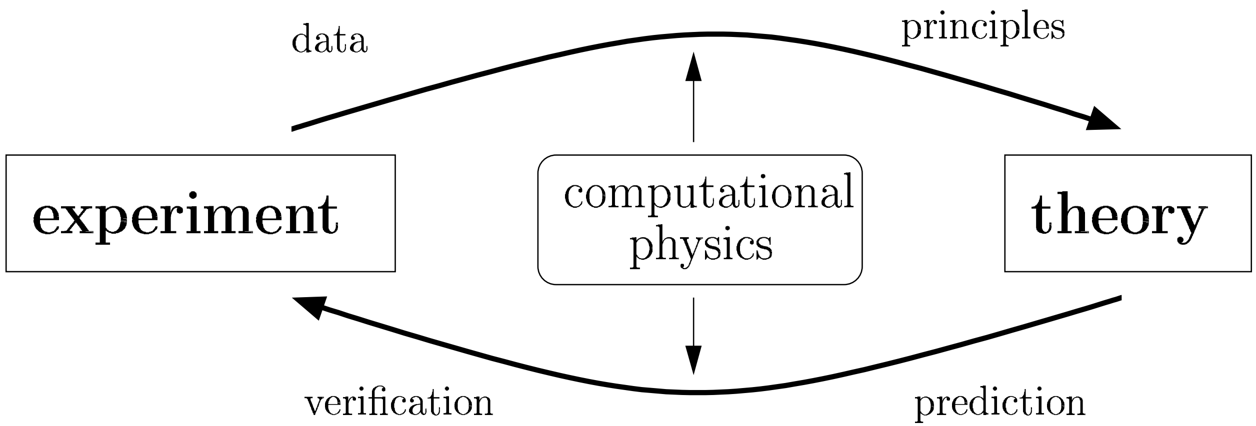
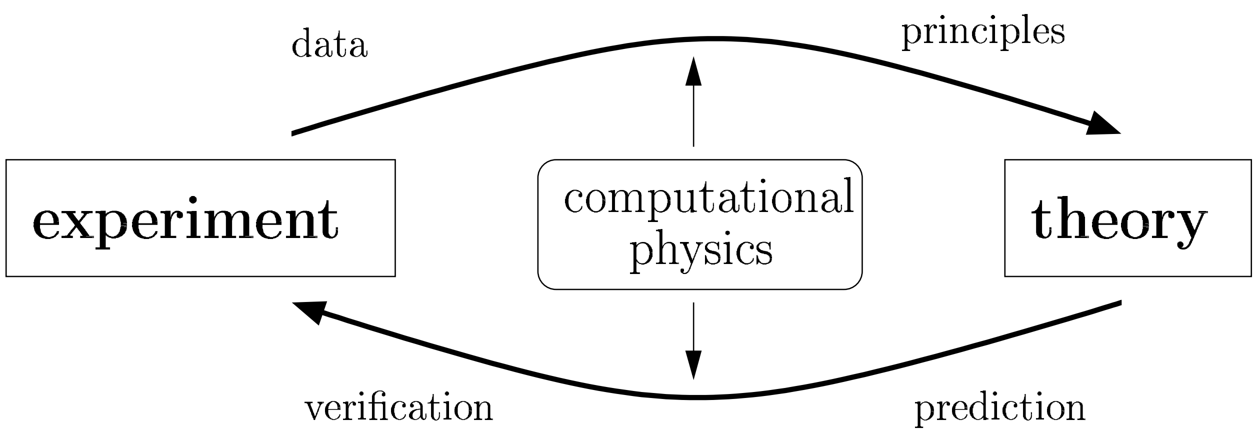
- warning
- computational techniques
- summary

motivation


data
principles
experiment
computational physics
theory
verification
prediction

motivation



challenge:

- precise mathematical theory
- often: solving theory's equations ab-initio is not realistic
- only a few models can be solved exactly

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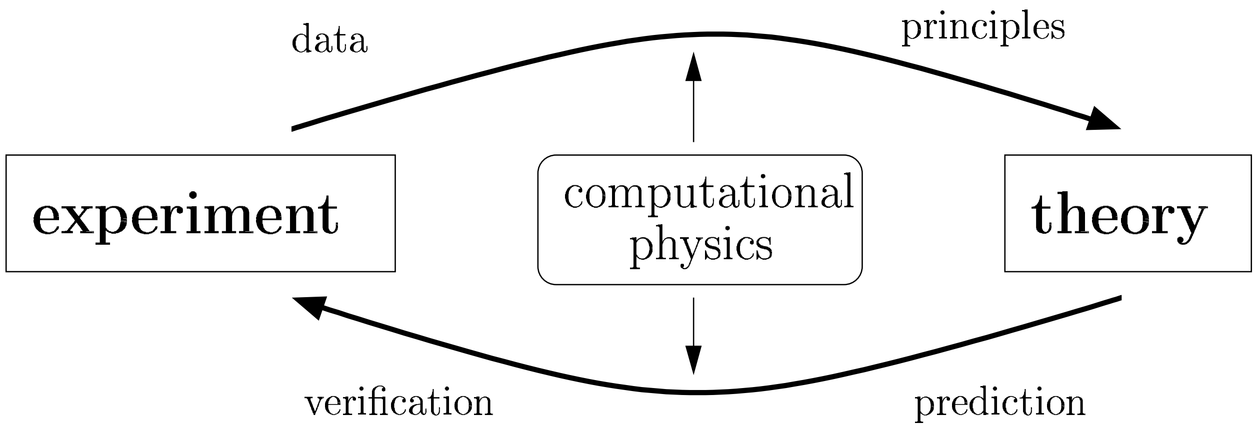

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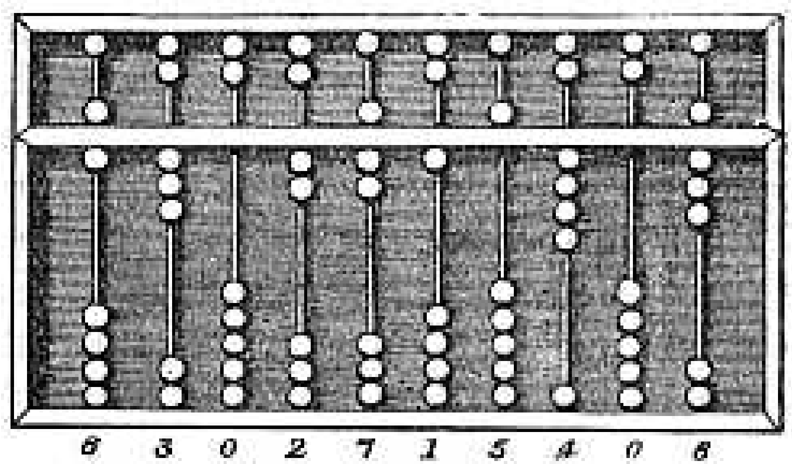
$\Rightarrow$ study and implementation of numerical algorithms

history of computing hardware



- $3000\,bc$: abacus - first calculating device

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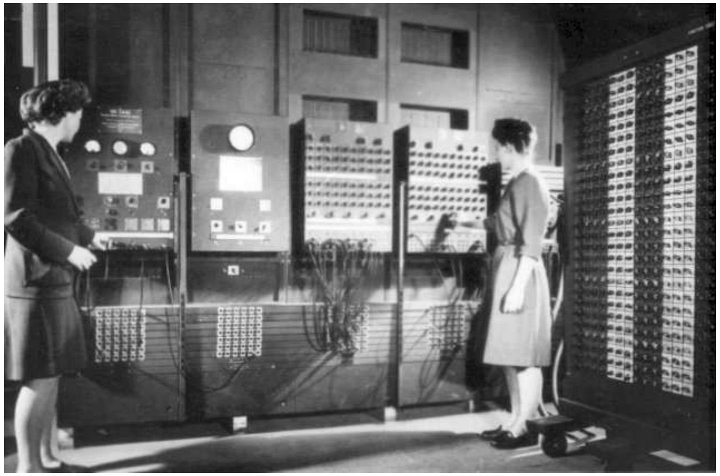

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 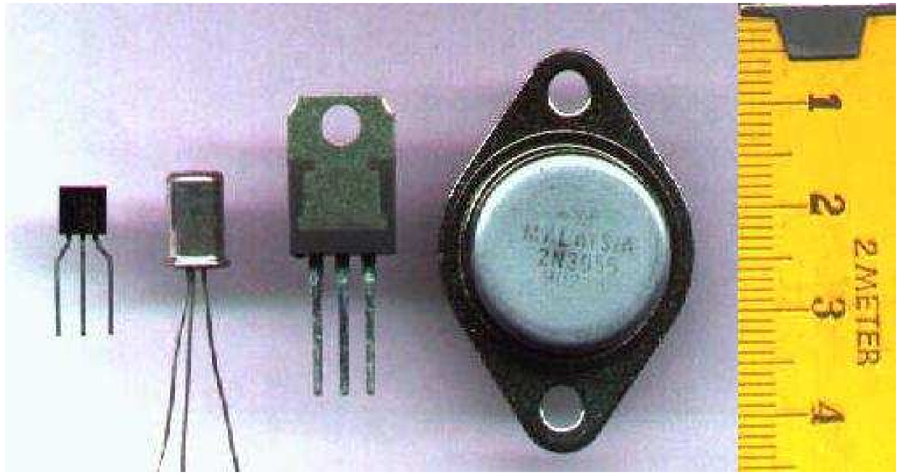

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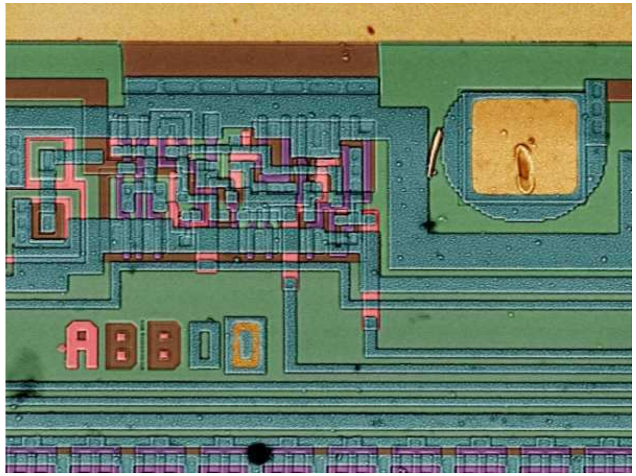

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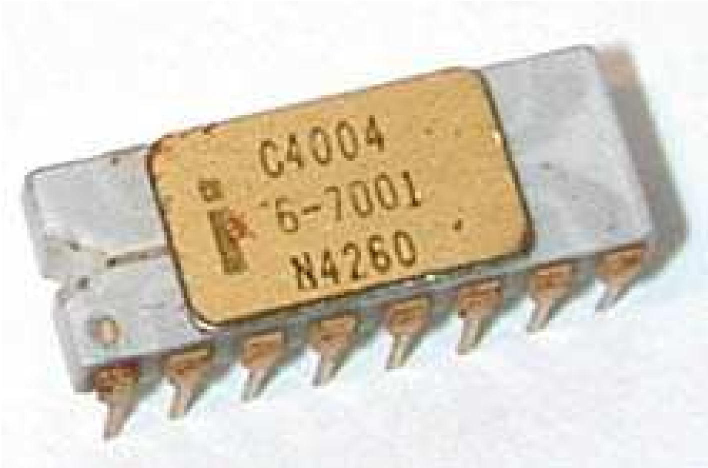

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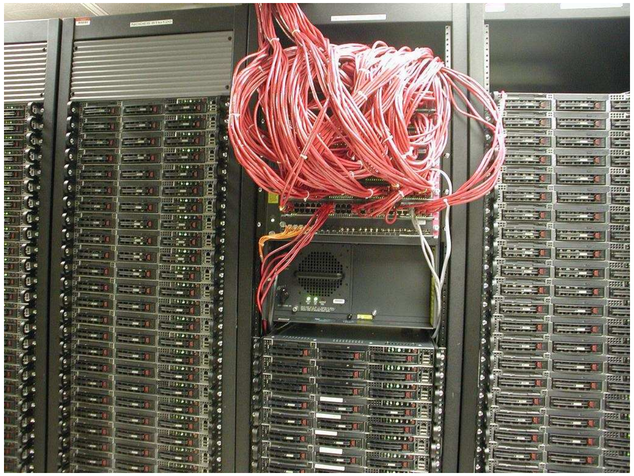

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- $1990/2000$: massive parallel computing

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- 1991: linux - open-source kernel

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  - machine independent, characteristic of used algorithm

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```
int fak(n) {
    int help=1;
    while(n>1) {
      help=help*n;
      n=n-1;
    }
return help;
}
```

computational techniques

- rough discretization
- solution of linear algebraic equations
- interpolation and extrapolation
- integration of functions
- evaluation of (special) functions
- monte carlo methods
- eigensystems
- spectral applications
- modeling of data
- ordinary differential equations
- two point boundary value problems
- partial differential equations

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http://www.nr.com/

first steps: rough discretization

- example: homogenous field of force $\vec{F} = (0, -mg)$

  equation of motion: $\vec{F} = m\vec{a} = m\frac{d^2\vec{r}}{dt^2}$

  initial condition: $\vec{r}(t=0) = \vec{r_0} = (x_0, y_0)$

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- algorithm using discretized time ($T = N\tau$):

  $x^1 = x_0;\quad y^1 = y_0;$

  $v_x^1 = v_{x_0};\quad v_y^1 = v_{y_0};$

  loop:

  $x^2 = x^1 + \tau v_x^1;\quad y^2 = y^1 + \tau v_y^1;$

  $v_x^2 = v_x^1;\quad v_y^2 = v_y^1 - g\tau;$

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- euler's method for solving o.d.e.

euler's method: error estimation

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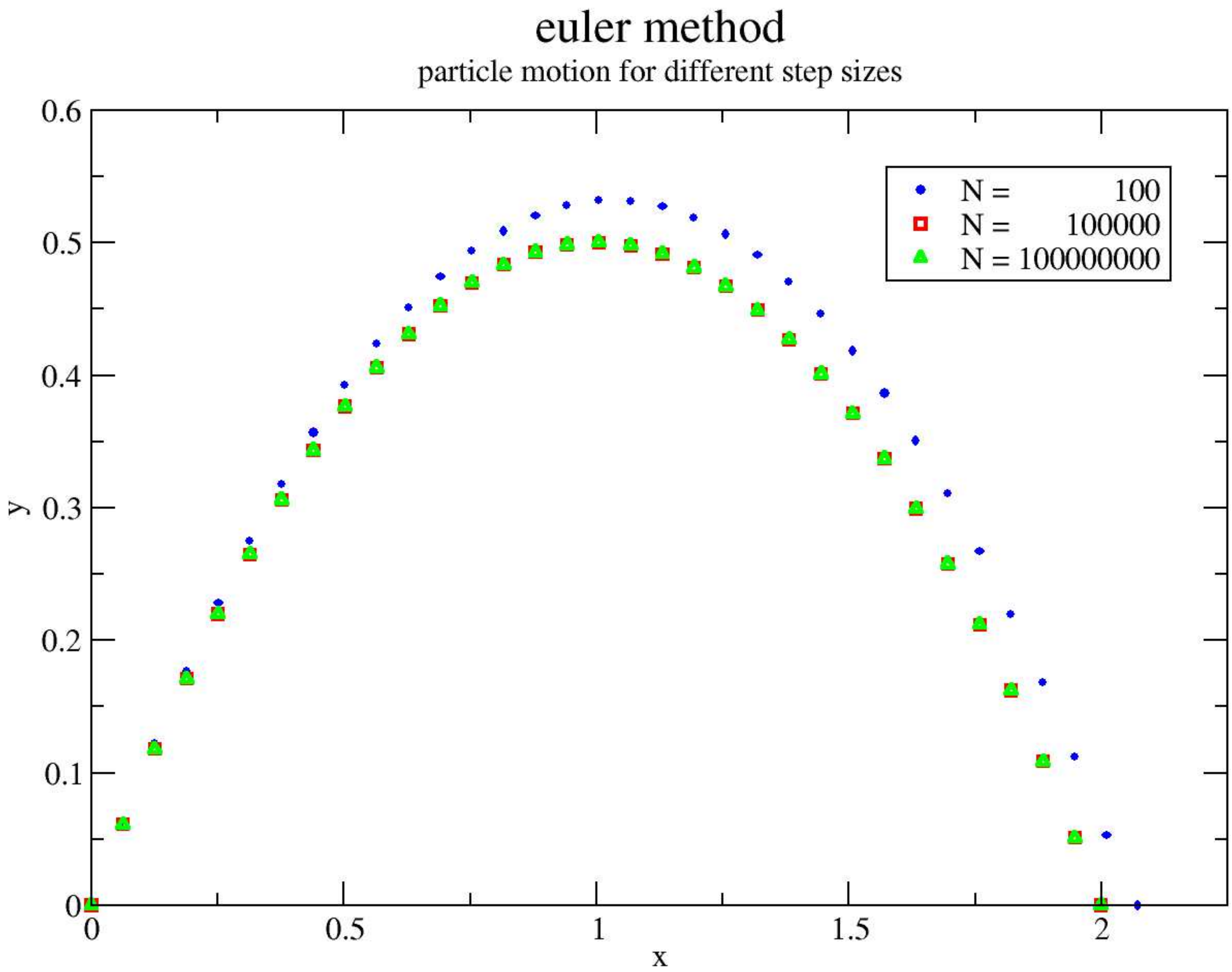
  - 32-bit: $\epsilon_m = 1.19 \times 10^{-7} \Rightarrow \tau \sim 3 \times 10^{-4}$

euler's method: accuracy



monte carlo methods

- algorithms for solving computational problems using random numbers

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  - no need fo simplifying assumptions

random number generator

linear congruential generator:

- $I_{j+1} = (aI_j + c)\, mod\, m$
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division by modulus $\Rightarrow$ uniform deviates :

$$p(x)dx = \begin{cases} dx & 0 \leq x < 1 \\ 0 & \text{sonst} \end{cases}$$

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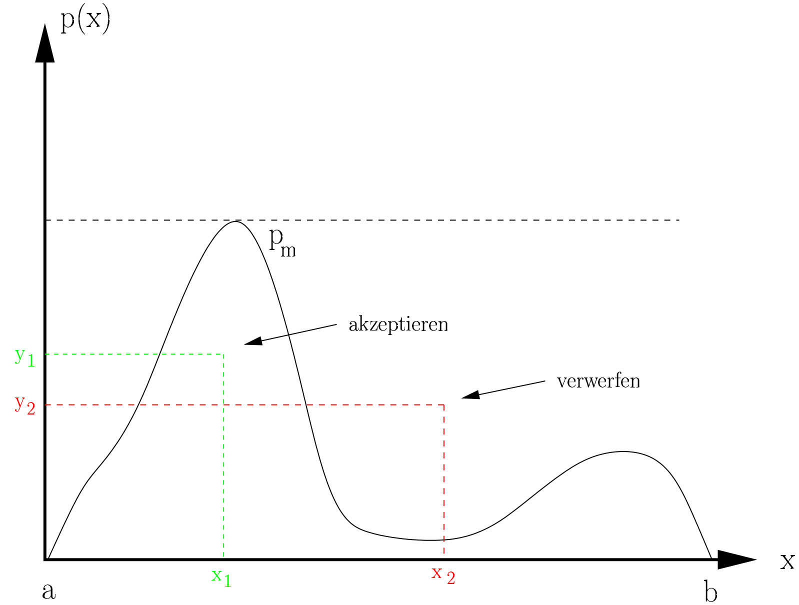

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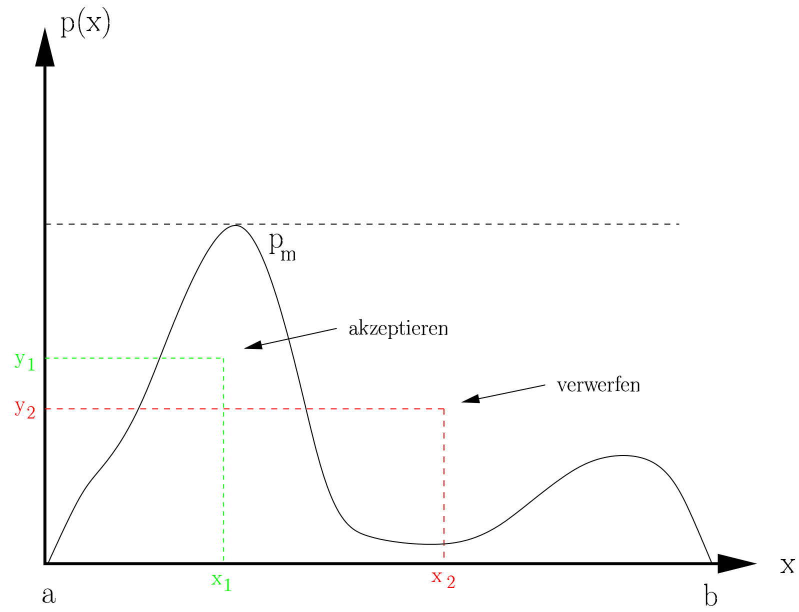

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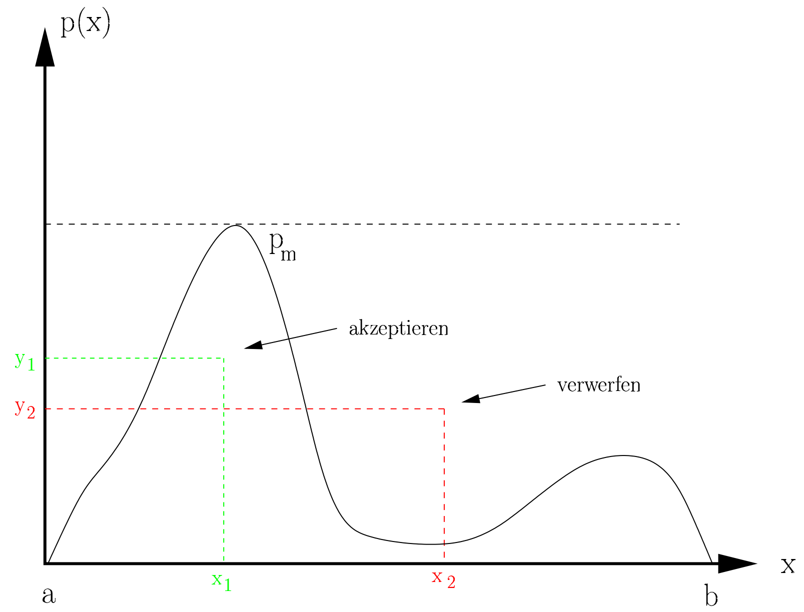

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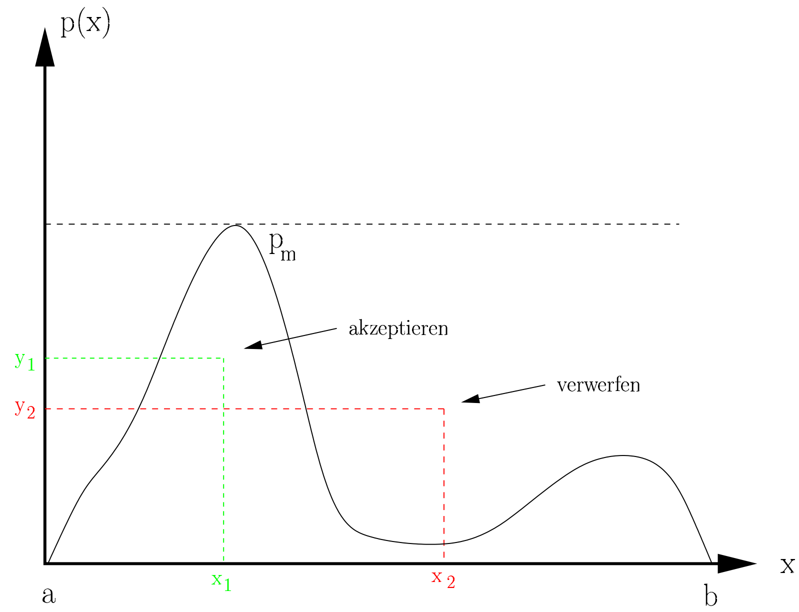
  - if $y \leq p(x)$ use x, else reject x



monte carlo integration

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$$\pi = \int_{-1}^{1} \int_{-1}^{1} p(x,y) dx dy \approx \frac{4}{N} \sum_{i=1}^{N} p(x_i, y_i)$$

$$\text{with } p(x,y) = \begin{cases} 1 & x^2 + y^2 \leq 1 \\ 0 & \text{sonst} \end{cases}$$

metropolis algorithm

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partition function:

$$Z = \sum_{i=1}^{N} e^{\frac{-E_i}{k_B T}} = Tr(e^{-\beta H})$$

metropolis algorithm

- importance sampling:
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- detailed balance

  sufficient condition for equilibrium:

  $$W(A \to B)p(A) = W(B \to A)p(B)$$

  $\Rightarrow \frac{W(A \to B)}{W(B \to A)} = \frac{p(B)}{p(A)} = e^{\frac{-\Delta E}{k_B T}}$

  with $\Delta E = E(B) - E(A)$

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  - flip spin if $r \leq e^{\frac{-\Delta E}{k_B T}}$

summary

- importance of computational physics
- things to keep in mind when doing computational physics
- euler's method for solving o.d.e.
- introduction to monte carlo methods