MA5710 Mathematical Modeling in Industry

Lecture – Part I

General Overview: Importance and Relevance Today, Approach & Hierarchy

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Modeling can be learned by doing, not by listening or reading.

Modeling is „metastrategic knowledge“
(see Elsbeth Stern: „Lernen“, Pädagogik 58(1)72006)

> *„Metastrategic knowledge emerges at best as a byproduct of the acquisition of content knowledge. Metastrategic knowledge is learnable, but only in exceptional cases direct teachable.“*

Find a good balance in teaching mathematics and exercising modeling.

The more mathematics we know, the better are the models.

Georg Christoph Lichtenberg (1742 – 1799)

"In order to find something,
you have to know that it exists."

Mathematics - Engine for the Economy

- *“Like no other science, mathematics helps our trade in solving all different kinds of problems - and exactly this universal applicability makes her the Queen of all disciplines“* (D. Zetsche, Daimler)

- *“Permanent changes determine the competition and its conditions. But yet there is one constant, which keeps everything in its nucleus together and is an important construc-tion element for innovation: Mathematics*“ (M. Jetter, IBM Germany)

- *“Without mathematics, successful riskmanagement is not possible“*
(Reto Francioni, German Stock Market)

- *“The management of enterprises without mathematics is like space flight without physics. Numbers are certainly not everything in the economy. But without mathe-matics almost everything is nothing“*
(H. Kagermann, SAP)

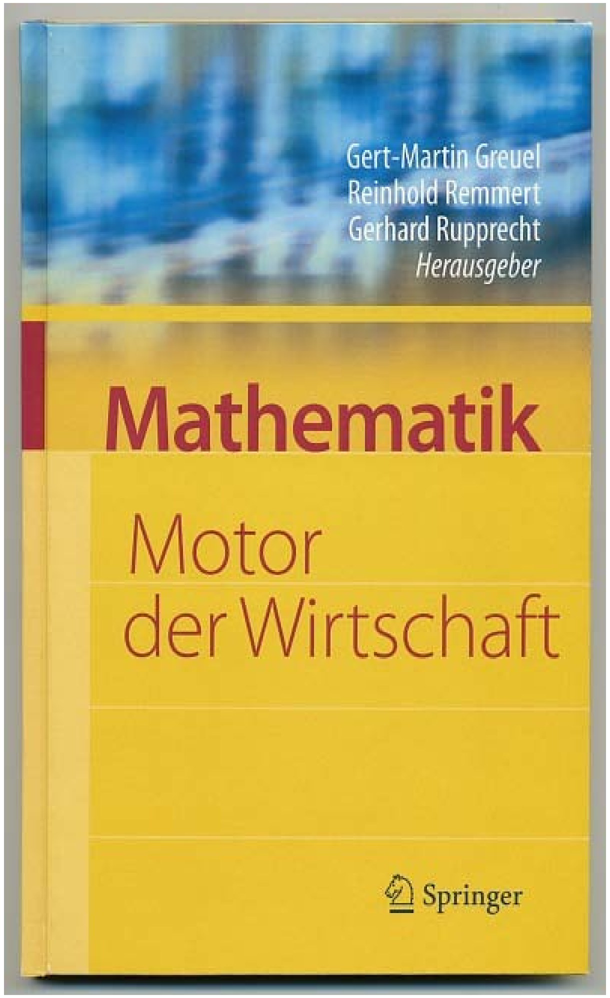
- *“Mathematics - that is the language of science and technology. Therefore, it is the driving force behind all high technology and the key discipline for all industrial nations. Without mathematics there is no progress and no technological innovation“*
(P. Löscher, Siemens)

Mathematics - Engine for the Economy

- edited by “Oberwolfach”,
Springer, April 2008

- Initiative of industry with respect to
“Year of Mathematics 2008“

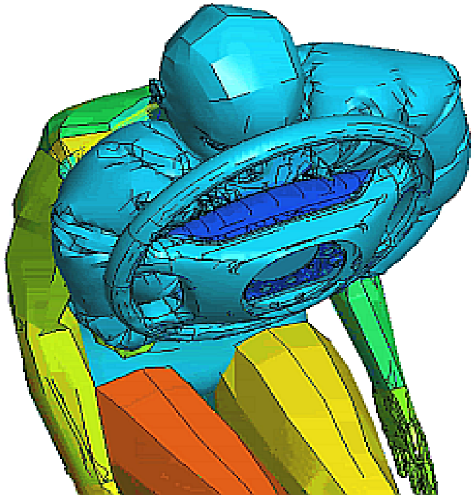
- Articles by the CEOs of
– Allianz – Bayer
– Böhringer Ingelheim – Daimler
– Deutsche Bank – Deutsche Börse
– Dürr – IBM
– Infineon – Linde
– Lufthansa – Münchner Rück
– RWE – SAP
– Siemens– TUI



Technology Fields (from Industry R&D perspective)

- Simulated Reality
- Optimization and Control
- Multiscale Models and Algorithms
- Risk and Decision
- Data, texts and Images

Simulated Reality in contrast to Virtual Reality



is created by

Modeling + Scientific Computing + Visualization

Modeling = Translation of the behavior of a real systems into mathematics.

The model has to be – as simple as possible

– as complex as necessary

Scientific computing = approximate evaluation o the models with help of a computer

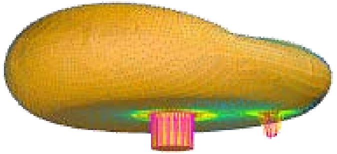
The evaluation has to be – as fast as possible (and sometimes even faster)

– as accurate as necessary

Examples for simulated reality

1. Motion of fibers or cables

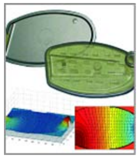
2. The behavior of vehicles - Multi body systems



3. Complex flows - in airbags, around fibers etc.

4. Cooling of glass

5. The behavior of filters



One needs knowledge in

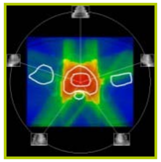
– Continuum mechanics – Differential geometry – stochastic
–Differ.-algebraic systems – CFD and acoustics – multiscale analysis
–Partial differential equations and integro-differential equations

Optimization and Control

is everywhere in industrial mathematics: It is easier to optimize in a simulated than in the real world.

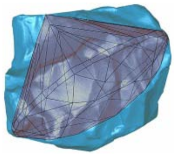
Examples

1. Inverse problems and parameter identification

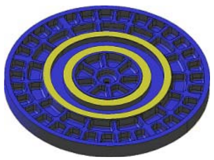


2. Multi criteria optimization as in radiotherapy planning

3. How to cut and polish gems optimally



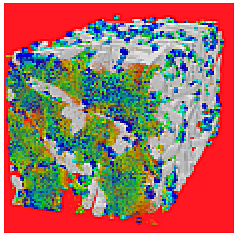
4. Optimal Shape Design



One needs knowledge in

– functional analysis – system and control theory
– multi criteria optimization – semi-infinite programming

Multiscale Models and Algorithms



belongs must often also to simulated reality.

It deals with

– considering “scenes” on different scales

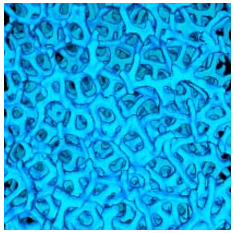
nano → micro → mezzo → macro

– dealing with transitions between the scales

– using different algorithms on different scales and combining them

Examples

– Filters – textiles
– composites – foam



One needs knowledge in

– Asymptotic analysis – homogenization – multigrid methods
– wavelets – stochastic geometry

Risk and Decision

tries to model risk in technical, economical and mainly financial (!) systems. Gives probabilities for the consequences of decisions.

Examples

1. The risk, that a fast train jumps out of tracks
2. Portfolio optimization
3. Option pricing

One needs knowledge in

- Stochastic differential equations
- martingales
- Stochastic optimization
- stochastic control
- Monte Carlo methods

Data, Texts and Images

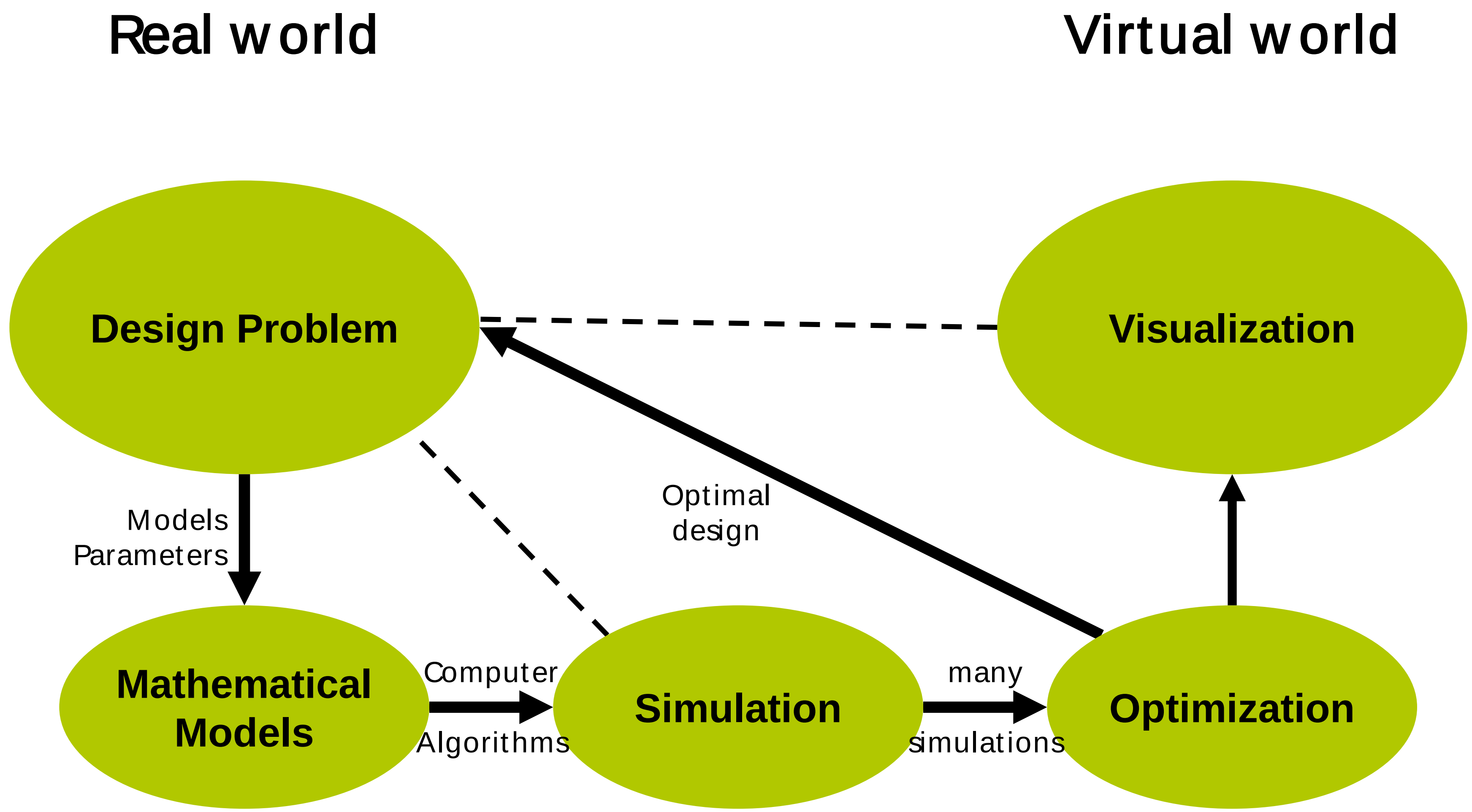
What to do with many data – observations, experimental results, measurements, if little theory is available?

Signal processing: Time Series Analysis

Input-Output-Systems: System theory, Data mining methods like neural networks, clustering etc.

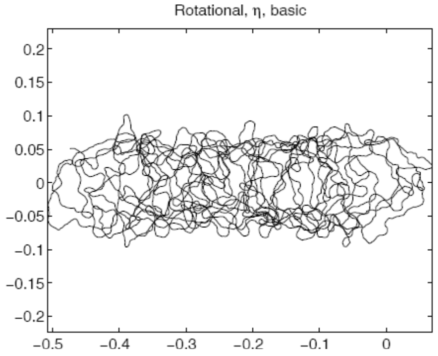
Discover order in data sets: Dynamical systems theory, …

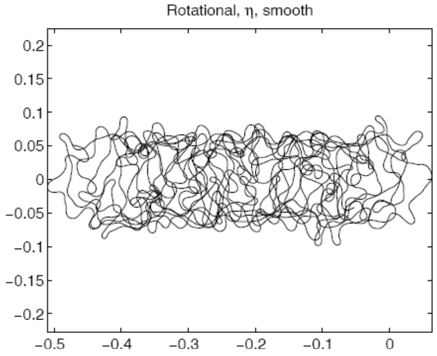
Image processing: Image compression, segmentation,…

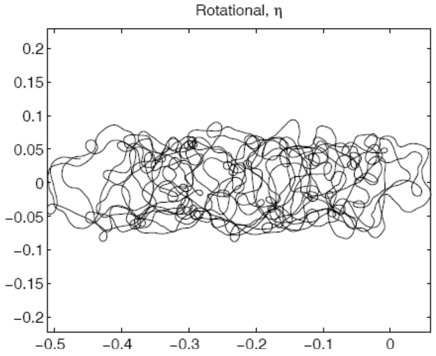

Real world
Virtual world
Design Problem
Visualization
Models
Parameters
Optimal
design
Mathematical
Models
Computer
Algorithms
Simulation
many
simulations
Optimization

Two Messages

- Keep in mind, that the model must be evaluated in a given time with given tools; this may be lead to a hierarchy of models







- Keep in mind, that the problem posed needs required slight change often, especially with respect to objective functions

Example 1: A Hierarchy of mathematical models for production processes of technical textiles

Granules

↓

Melting and
spinning of fibers

↓

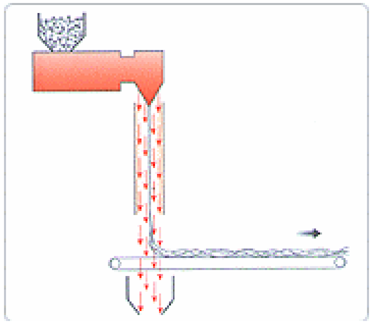
Curling of fibers
through turbulences

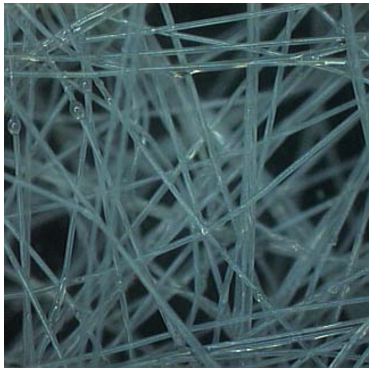
↓

Deposition at the
conveyor belt

↓

Non-wovens

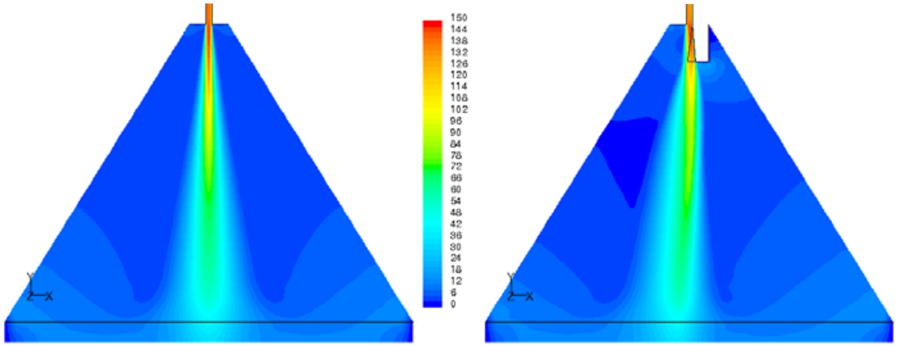




The input – output system

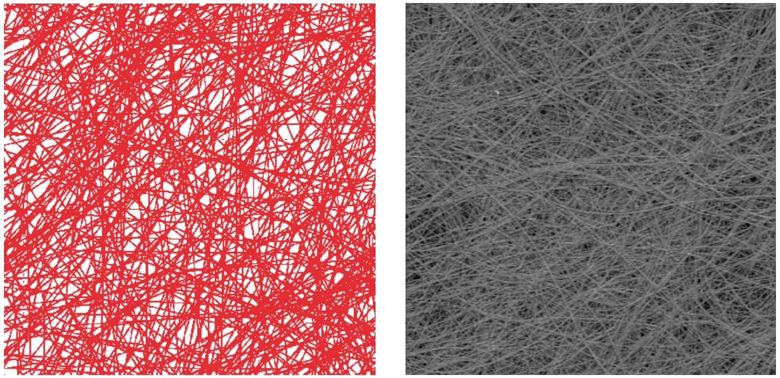
Input:

- fluid data
- geometry
- (material)



Output:

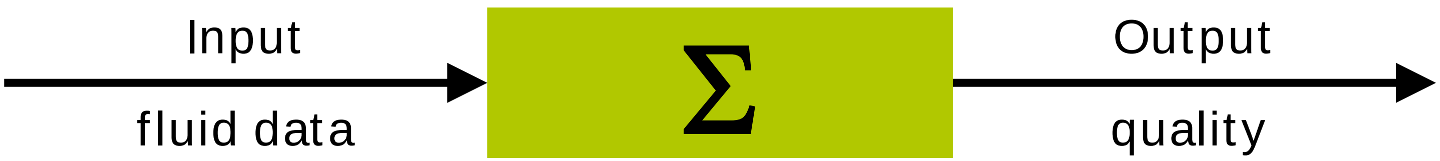
- quality of the fleece



virtual fleece real fleece

How to measure quality?

System theoretical description



Σ = class of mappings

Little theory ➔ class contains many parameters ➔ many observations are necessary in order to identify these parameters

Class: linear control systems, neural networks etc.

Black box models

Disadvantage: Only the prediction of already existing systems is possible

Much theory ➔ class contains few, i.g. measurable parameters

Class: Equations of continuum mechanics

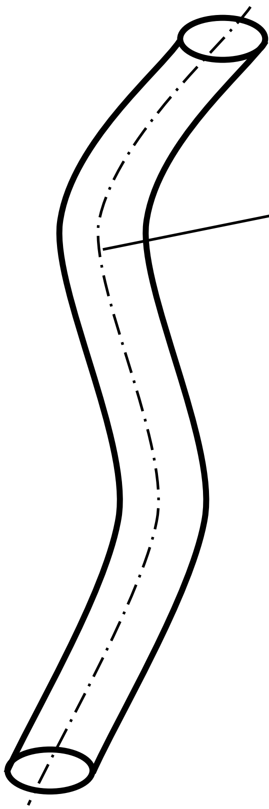
White box models

Disadvantage: Very costly numerical evaluation

In-between: **Grey box models**

The »almost white« model

Theory of Elasticity:



Rod theory (1d)

$\underline{r}(s,t)$

arc length   time

$$\partial_{tt}\underline{r} = \partial_s(T\partial_s\underline{r}) + D_s\underline{r} + f$$

$\|\partial_s\underline{r}\| = 1$ Incompressibility

$f =$ Air forces

Theory of Fluids

Navier-Stokes Equations which contain air forces f

$f =$ depend on the relative velocity

$\partial_t \underline{r} - u$

The numerical solution of Navier-Stokes in 3d with higher Reynolds numbers (10^4) is not feasible!

➔ This „almost white model" is not applicable.

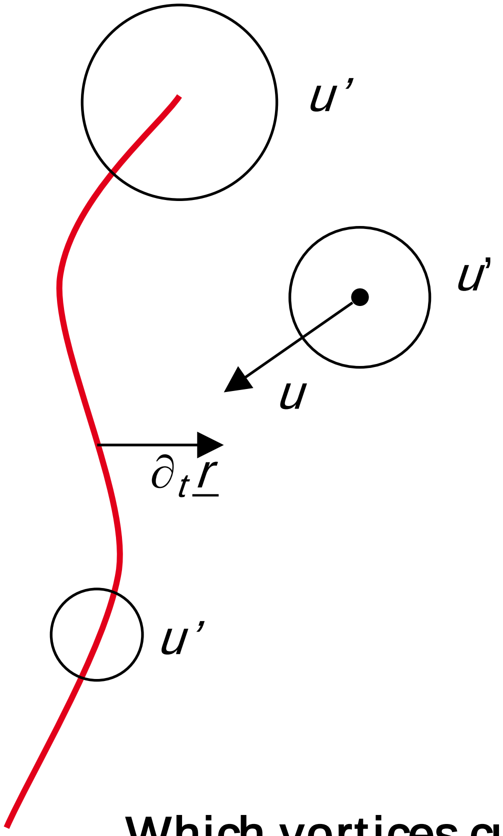
Turbulence models (as k-ε model) need 2-3 hours per fiber: Still not applicable, since we have 1000 fibers.

➔ Further simplifications are needed, i.e.
search for small parameters + asymptotic analysis.

The length scales of the flow

fiber length $L \cong$ typical length 1

fiber thickness $\sim \sqrt{A}$

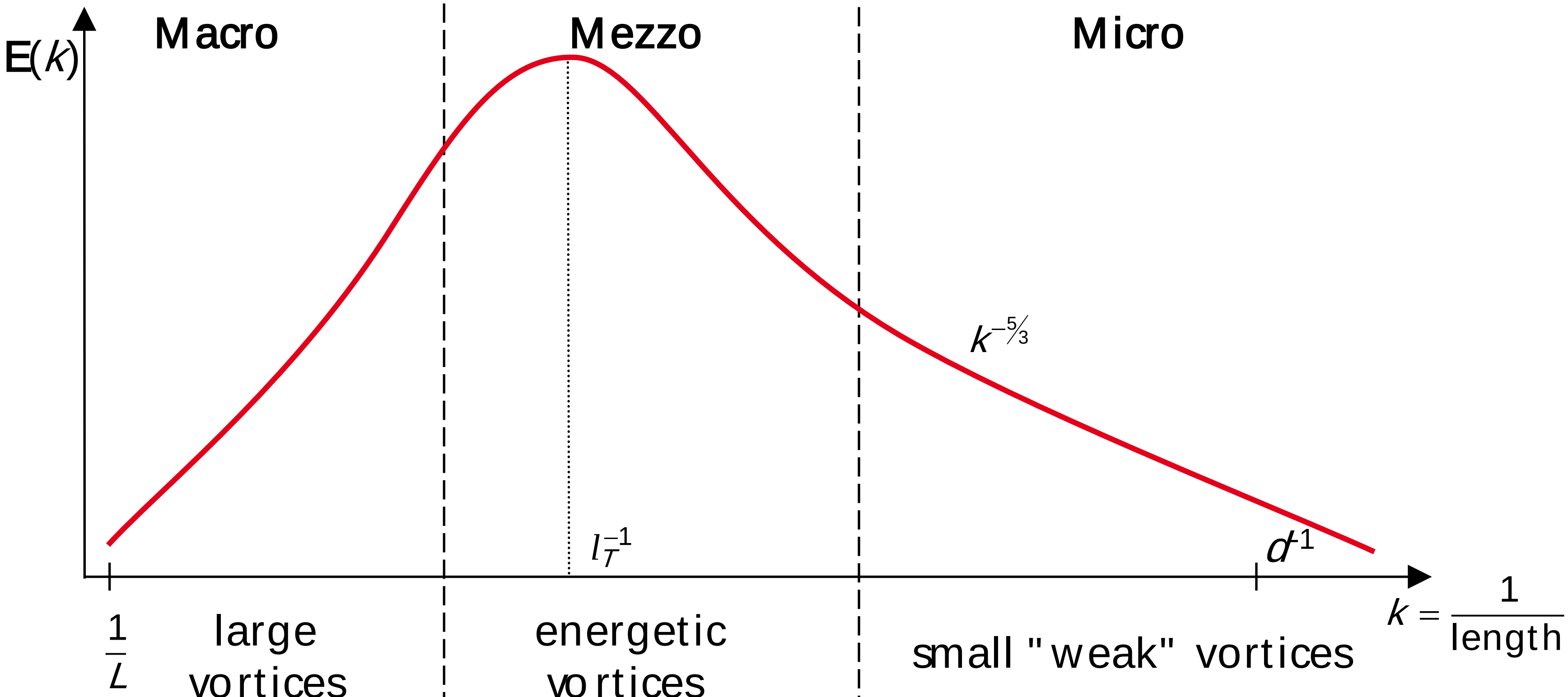


Turbulence contains vortices of different sizes, which interact with the fiber.

The vortices have different energies, depending on their diameters.

Which vortices curl the fibers?

Kolmogorov-theory



Macro	Mezzo	Micro
Motion of fibers is determined by the bulk velocity	Interior forces and turbulent forces in equilibrium	No interaction

The asymptotic limit

The fundamental scale is l_T, which we compare with the length L of the fibre

$$\delta = \frac{l_T}{L} \approx 10^{-3}$$

Asymptotic limit: $\delta \to 0$

Then turbulence forces $\xrightarrow{\delta \to 0}$ white noise

Now, a simulation can be made, but takes still several hours for realistic situations

$\to$ No optimal process design is possible

Still too costly (2 – 3 hours)

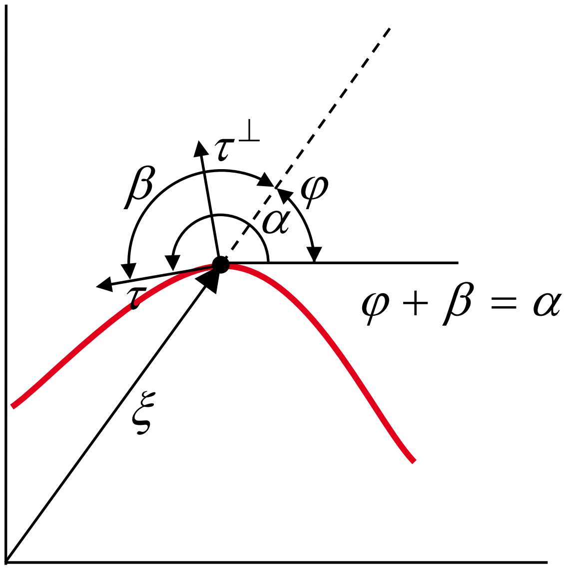
We have hundreds of fibers!

Further simplification

is needed = The **»grey model«** for the deposition

Non-moving conveyor belt „Impact point" of the fiber at the belt = $x(s)$

fiber incompressible è $t = s$



$$\dot{\xi} = \tau \quad , \quad \dot{\alpha} = -b(\|\xi\|) \underbrace{\frac{\xi}{\|\xi\|} \cdot \tau^{\perp}}_{\cos(90-\beta)=\sin\beta} + \tilde{A}dW$$

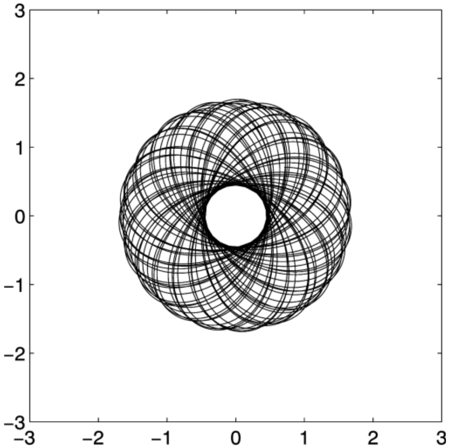
$0 \le \beta \le \pi \quad \Rightarrow \quad \sin\beta \ge 0 \quad \Rightarrow \quad \alpha$ decreases

$\Rightarrow$ The motion is turned towards direction ξ depending on b

$\tilde{A}$ = Amplitude of the projection of the turbulence

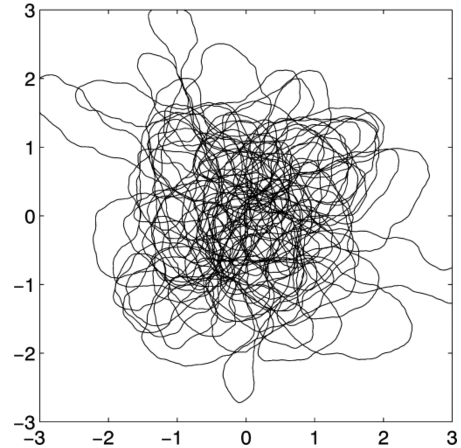
Influence of the turbulence

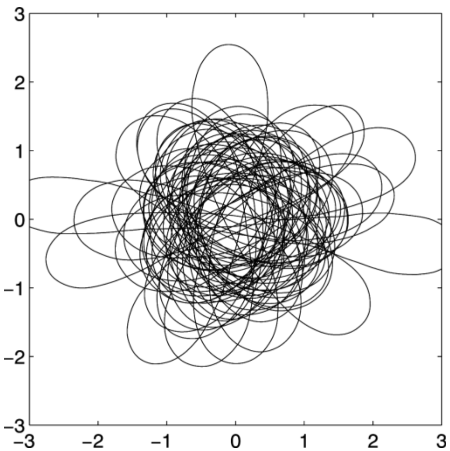
conveyor belt doesn´t move, $b(\|\xi\|) = 1$



$\tilde{A} = 0$

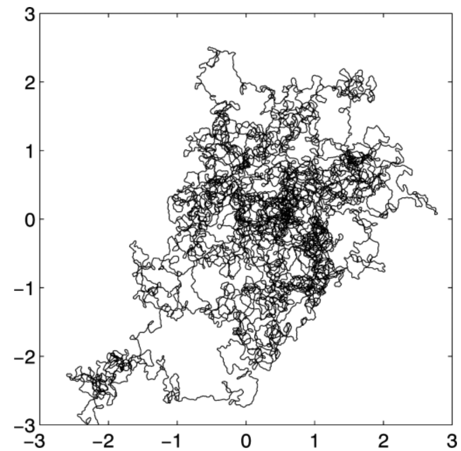
$\tilde{A} = 1$





$\tilde{A} = 0{,}1$

$\tilde{A} = 5$



$\tilde{A}$ and b are identifiable parameters.

What should we learn from this example:

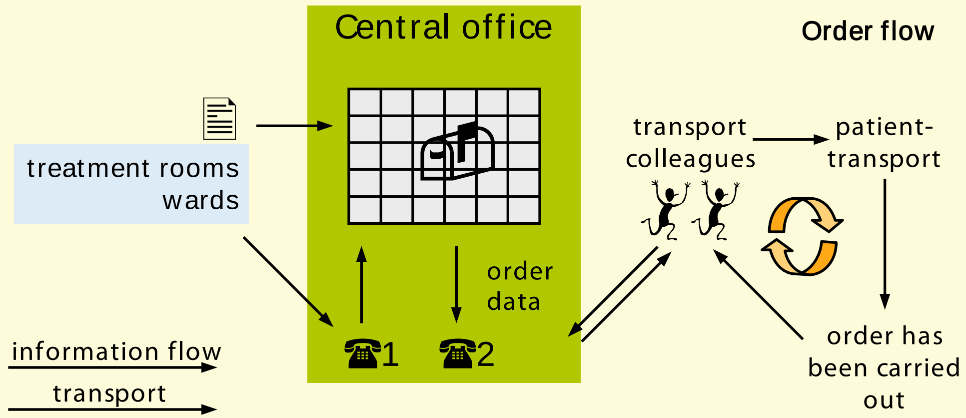
- That there is not **one** model, that there might be a hierarchy of models
- how we get simpler models from complex models (f.e. by asymptotic analysis)
- that we may use complex models to identify parameters in simpler models
- that models in order to be useful must be evaluated in a given time with given tools; therefore, efficient algorithms are very important too
- that models should be as simple as possible, but also as complex as necessary!

A never-ending challenge:

- Model and simulate the complete chain from production process to the final product
- Inverse problem: How to control the production to get an optimal product?

  Example: from filter features back to the spinning process

Example 2: Transport of Patients in Hospitals

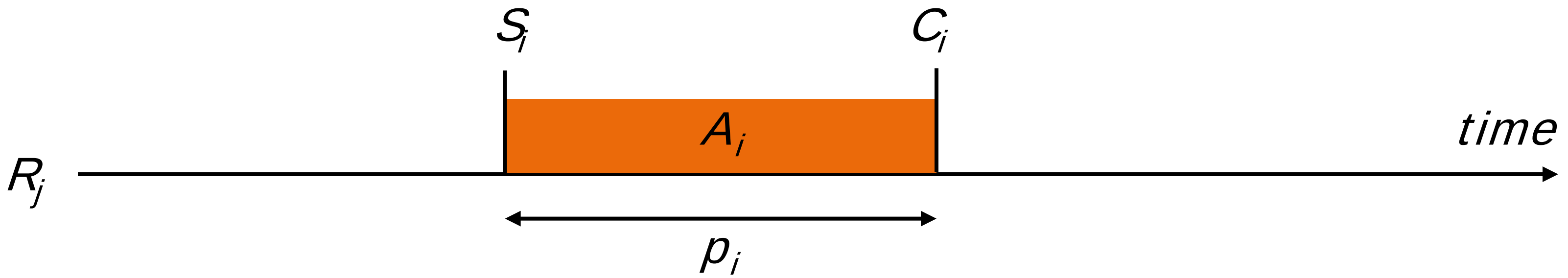


Scheduling – Activities and Resources

Activity A_i

- p_i – processing time
- S_i – start time (to be determined)
- C_i – completion time
- $C_i = S_i + p_i$

Resource R_j (can be machine, worker,…)

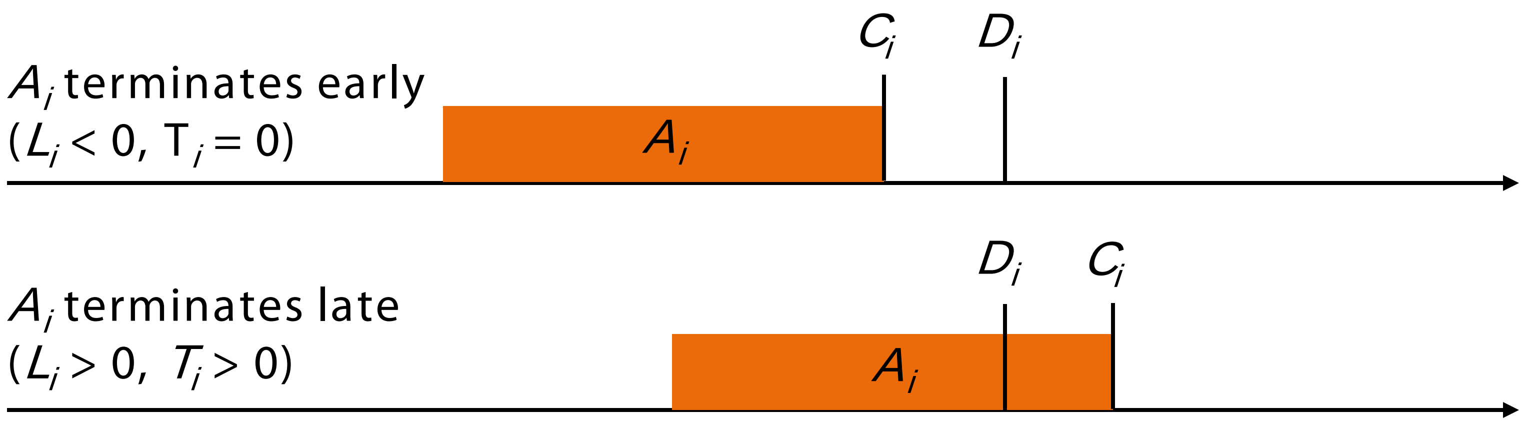


Scheduling – Lateness and Tardiness

Activity A_i

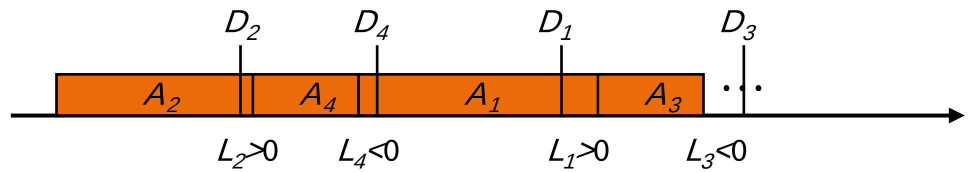
- D_i – due date

- $L_i = C_i - D_i$ lateness
- $T_i = \max(L_i, 0)$ tardiness



Scheduling – some examples for objective functions

Activities $A_1, A_2, \ldots A_n$



Task:
Schedule activities on a single resource (determine sequence) such that …

- $\max_i L_i$ is minimized → EDD rule is optimal („earliest due date")
- $\sum_i L_i$ is minimized → SPT rule is optimal („shortest processing time")
- $\sum_i T_i$ is minimized → problem is *NP*-hard, no rule exists

EDD rule: sort $A_1, A_2, \ldots A_n$ in non-decreasing order of due date

SPT rule: sort $A_1, A_2, \ldots A_n$ in non-decreasing order of processing time

Multiple resources

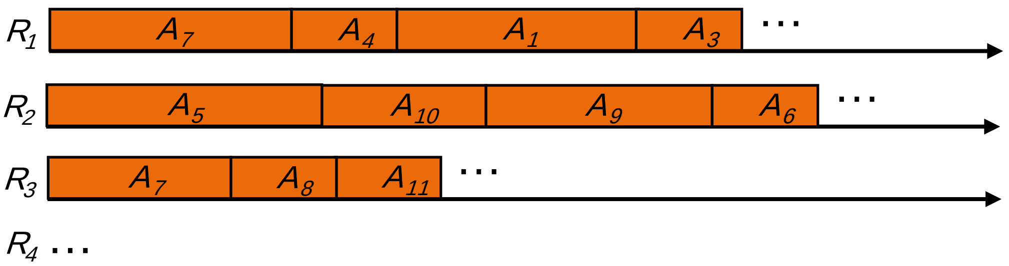
Activities $A_1, A_2, \ldots A_n$

Resources $R_1, R_2, \ldots R_m$

Tasks:

(1) Assign activities to resources

(2) Schedule activities on each resource



Example – Transport of Patients in Hospitals

Typical transport task:

- Bring patient Smith from ward to X-ray department for examination
- Performed by transport personnel

Model:

- Transport tasks – activities $A_1, A_2, \ldots A_n$
- Transport personnel – Resources $R_1, R_2, \ldots R_m$

Dispatcher:

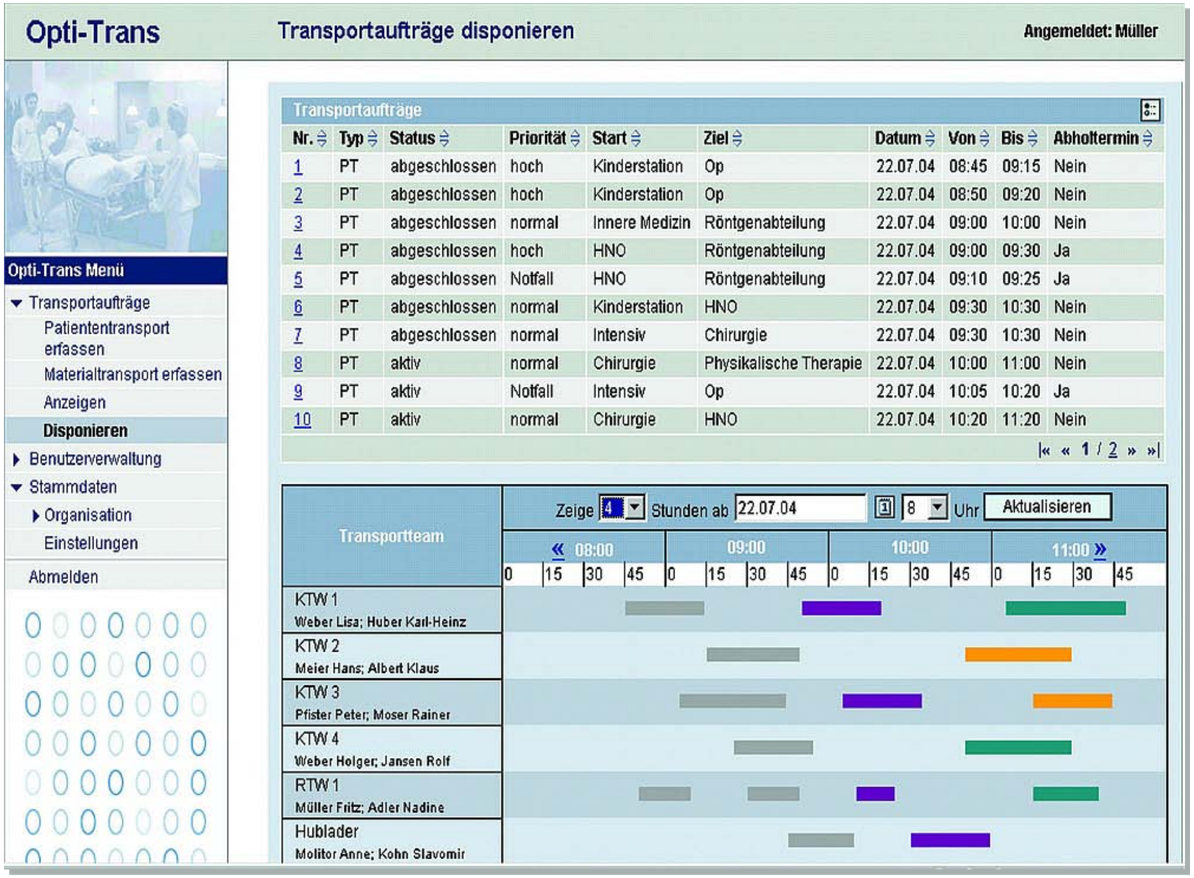
- Assign tasks to personnel
- For each worker determine sequence of tasks

Dispatching of transport tasks with classical media

- telephone
- paper
- pencil
- …

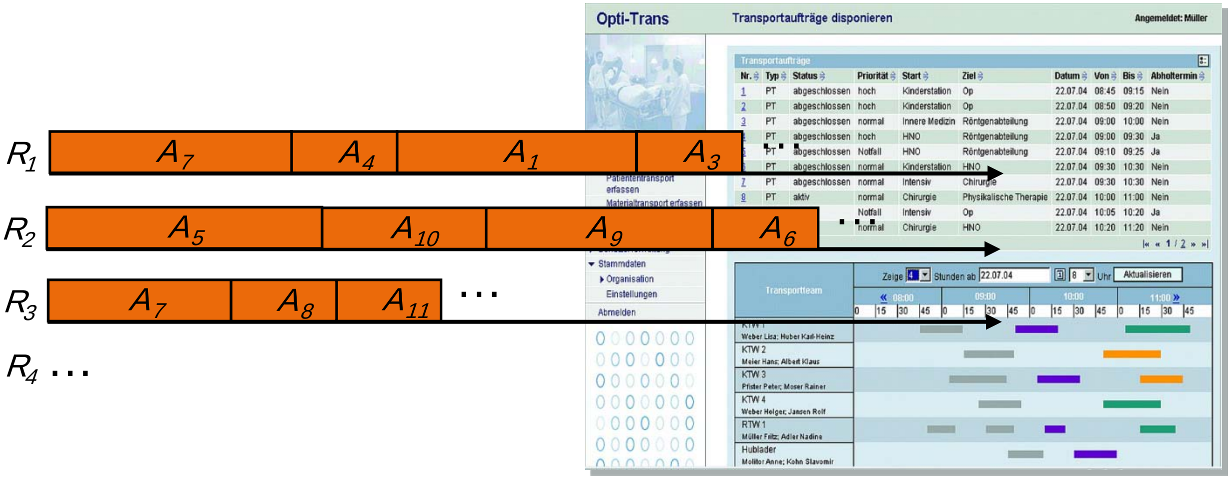
Dispatching of transport tasks with computer system

- Opti-TRANS®
- the whole process is software based
- dispatching algorithms



Objectives in Opti-TRANS® dispatching algorithm

- maximize timeliness (ideally lateness = 0 for all tasks)
- maximize resource utilization (avoid long ways between two tasks)
- balance workload on resources



Balancing of workload for human resources

- very important for transport personnel
- appropriate measure for workload?
  - e.g. number of tasks
  - e.g. total processing time

- human resources are not always available (working times, breaks,...)
- workload measure has to be neutral to times of absence

- set of transport tasks changes dynamically – frequent re-planning is necessary
- workload measure has to be stable over re-plannings

What should we learn from this example:

- How scheduling processes may be modeled
- that one needs many personal contacts, when human decisions are involved
- that optimization problems very often have not only **one** objective function: Multicriteria Optimization

Inverse Problems

Inverse Problems are concerned with finding causes for an observed or a desired effect.

Identification or Reconstruction, if one looks for the cause of an observed effect.

Control or Design, if one looks for a cause of an desired effect.

Example 1:

$$Af(x) = \int_0^x I(x-t)\, f(t)\,dt = g(x)$$

Assume: $I \equiv 1$ $\quad Af(x) = \int_0^x f(t)\,dt = g(x)$ $\quad$ If:

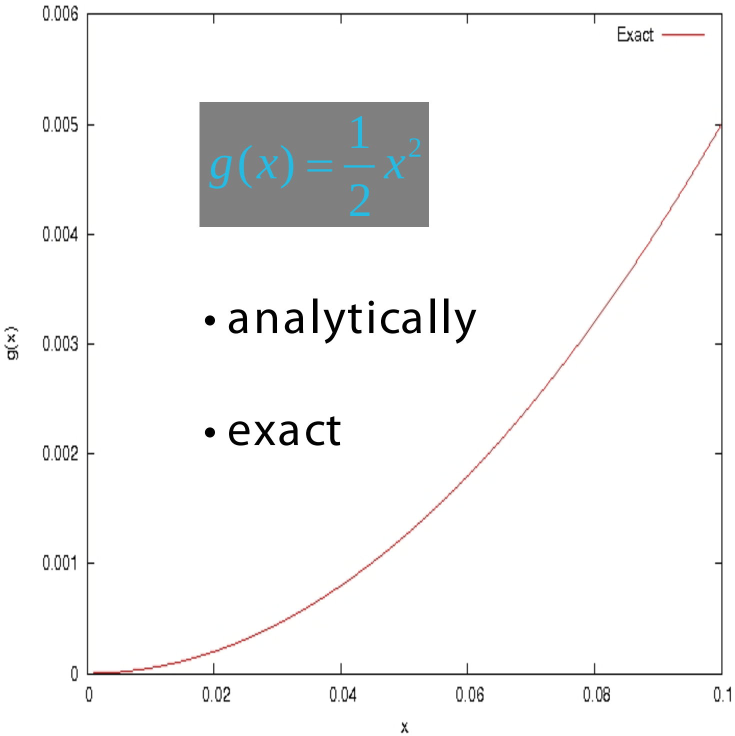
- Continuous differentiable

$$g(0) = 0$$

Solution: $\boxed{f(x) = g'(x)}$

Example 1:

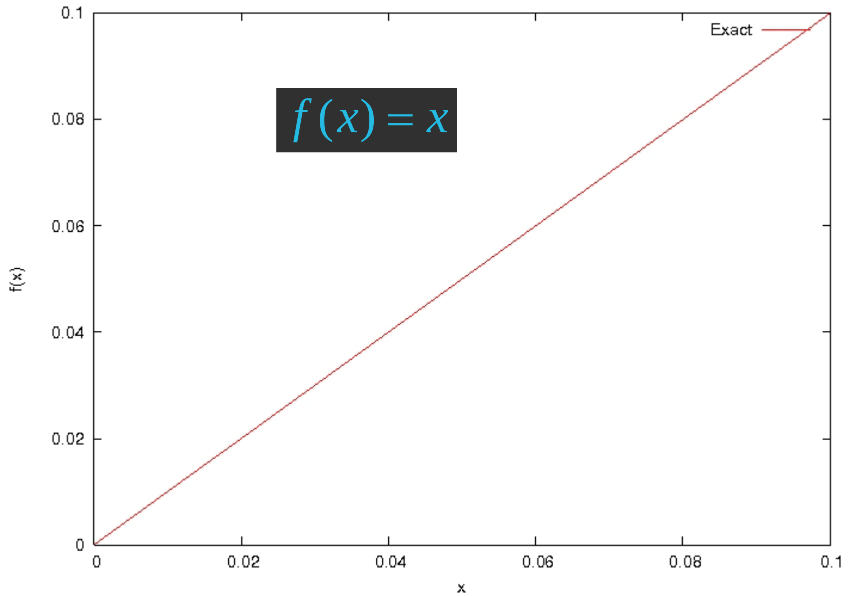
Given is:



$$g(x) = \frac{1}{2} x^2$$

- analytically
- exact

We find:

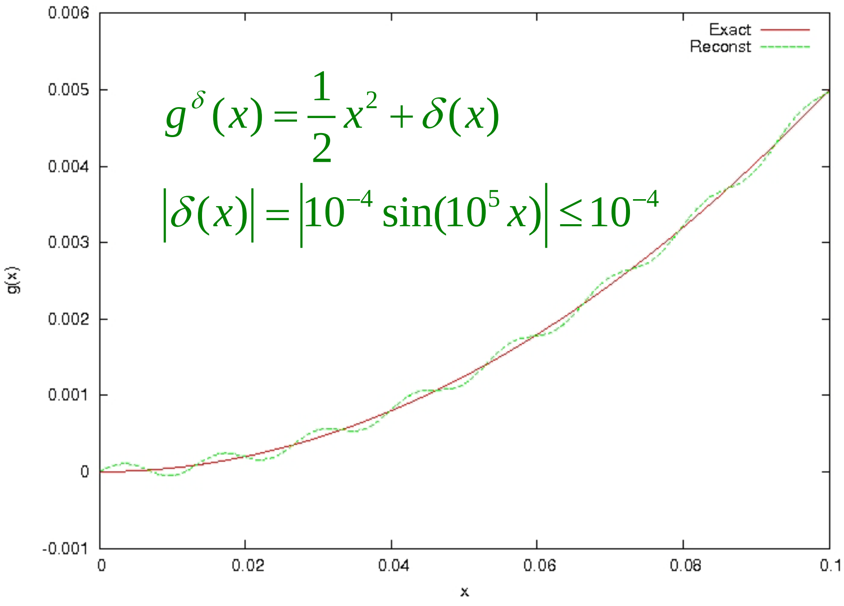


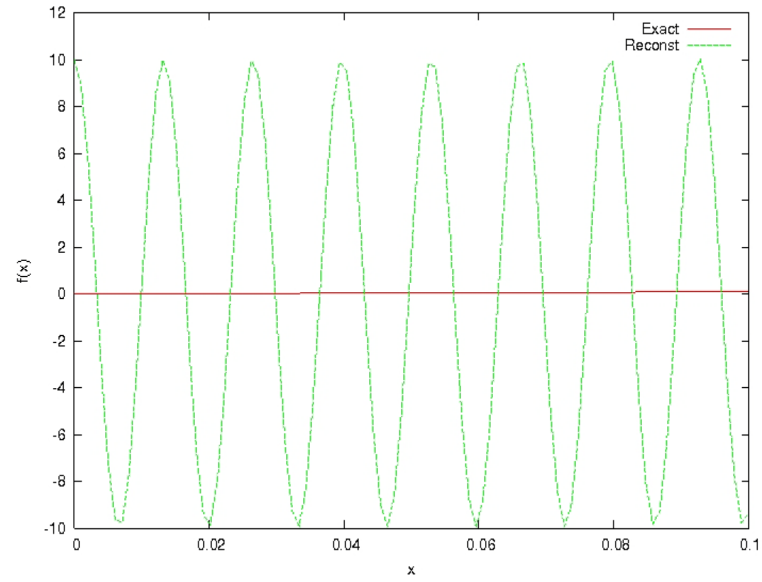
$$f(x) = x$$

A small error in the measurement causes a big error in the reconstruction!

$$g(x) = \frac{1}{2}x^2$$

$$f(x) = x$$





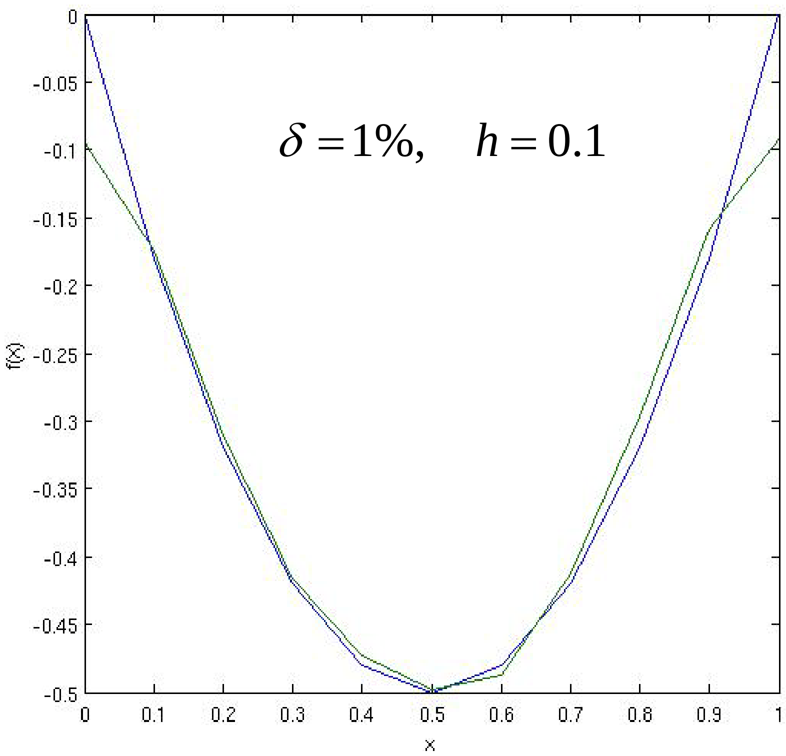
Numerical Differentiation

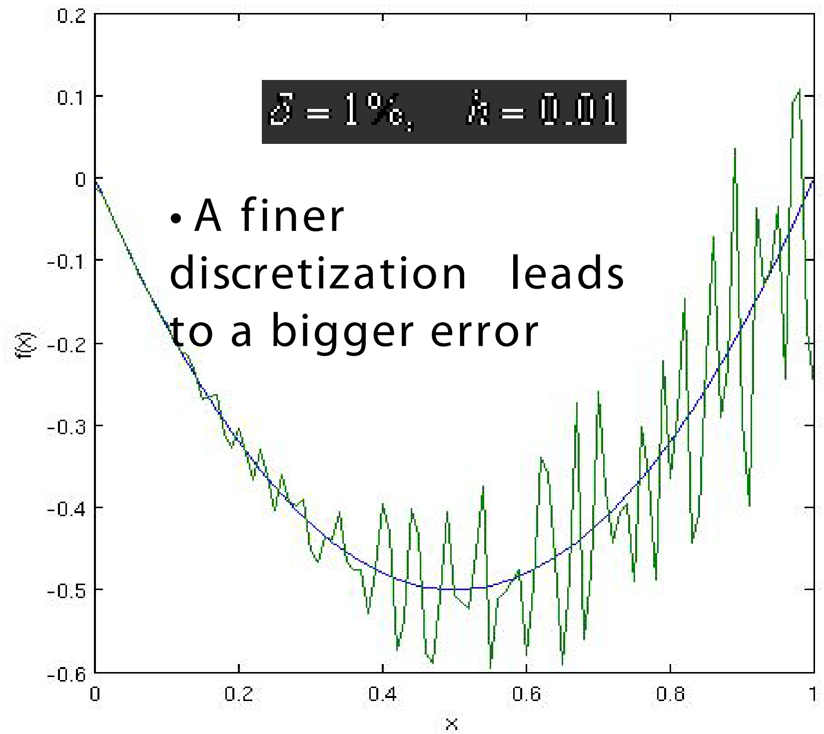
- In practice the measured data are finite and not smooth

$$g_i = g(x_i), \quad h_i = x_i - x_{i-1}, \quad i = 1, 2, \ldots, n \longrightarrow g_i^\delta$$

$$f_i = f(x_i) \longrightarrow f_i^\delta = D_h g_i^\delta = \frac{g_{i+1}^\delta - g_{i-1}^\delta}{2h}$$

Example 1: Numerical Differentiation

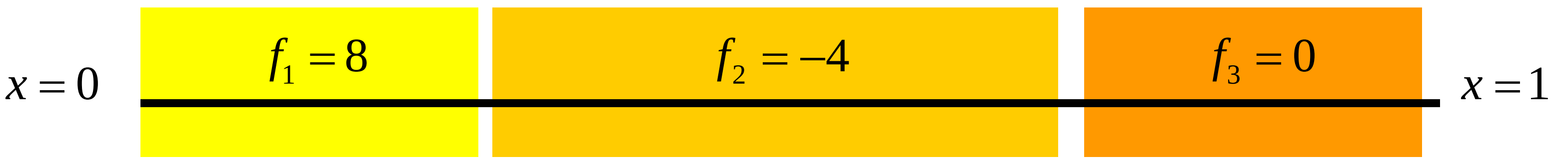




- A finer discretization leads to a bigger error

Inverse Problems

Example 2:



$\sigma_1 = 1.99999801$ $\quad\sigma_2 = 1.99\cdot 10^{-6}$ $\quad\sigma_3 = 1.0\cdot 10^{-8}$

$$\frac{\partial}{\partial x}\left(\sigma(x)\frac{\partial u}{\partial x}(x)\right) = -f(x), \quad 0 < x < l,$$

$$\sigma(0)\frac{\partial u}{\partial x}(0) = 0, \quad -\sigma(l)\frac{\partial u}{\partial x}(l) = \beta u(l)$$

$$\longrightarrow \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1.000001 & -0.000001 \\ 0 & -0.000001 & 1.000001 \end{pmatrix}\begin{pmatrix} u_1 \\ u_2 \\ u_2 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$$

exact solution: $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$

Reconstruction: $\begin{pmatrix} u_1 \\ u_2 \\ u_2 \end{pmatrix} = \begin{pmatrix} 20001.03 \\ 20000.02 \\ 0.000002 \end{pmatrix}$

Inverse Problems

A common property of a vast majority of Inverse Problems is their **ill-posedness**

A mathematical problem is **well-posed**, if

1. For all data, there exists a solution of the problem.
2. For all data, the solution is unique.
3. The solution depends continuously on the data.

A problem is **ill-posed** if one of these three conditions is violated.

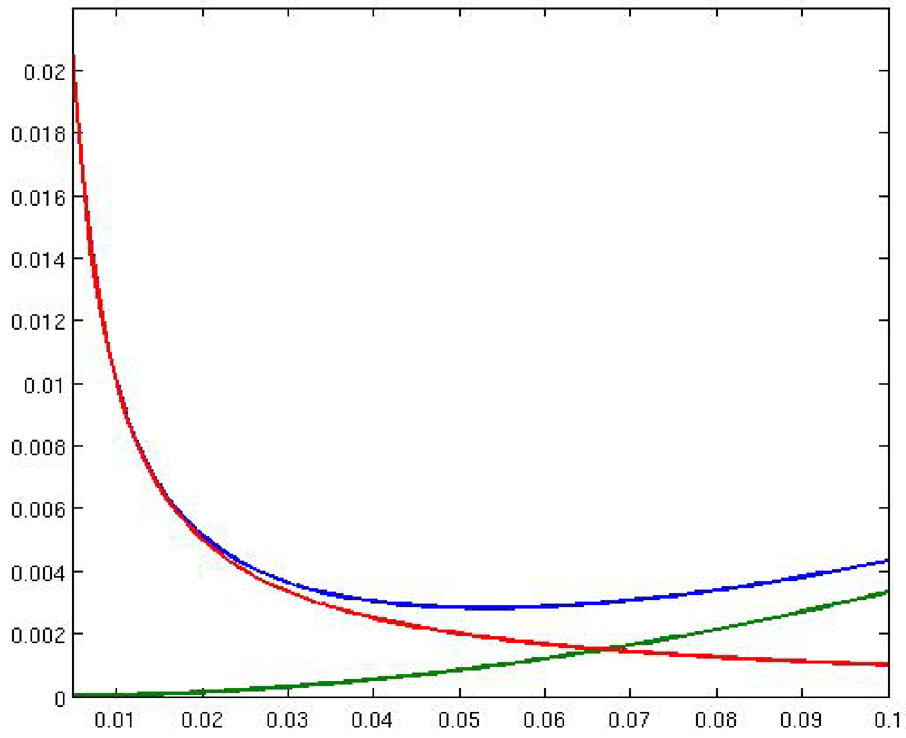
J. S. Hadamard
(1865-1963)

Inverse Problem

What is the reason for the ill-posedness?

Example 1:

$$\left|D_h g^\delta - f\right| \le \frac{h^2}{6}\|f''\|_\infty + \frac{\delta}{h}$$



Step size must be taken with respect

to the measurement error

Inverse Problems

What can be done to overcome the ill-posedness? → **Regularization**

- Replace the ill-posed problem by a family of neighboring well-posed problems

Regularization Methods

1. Truncated Singular Value Decomposition
2. Tichonov (Lavrentiev) Regularization
3. Landweber Iteration
4. Classical Tichonov Regularization