Fraunhofer Institut Techno- und Wirtschaftsmathematik

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Mathematics as a Technology: Challenges for the next 10 Years

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Vorwort

Das Tätigkeitsfeld des Fraunhofer Instituts für Techno- und Wirtschaftsmathematik ITWM umfasst anwendungsnahe Grundlagenforschung, angewandte Forschung sowie Beratung und kundenspezifische Lösungen auf allen Gebieten, die für Techno- und Wirtschaftsmathematik bedeutsam sind.

In der Reihe »Berichte des Fraunhofer ITWM« soll die Arbeit des Instituts kontinuierlich einer interessierten Öffentlichkeit in Industrie, Wirtschaft und Wissenschaft vorgestellt werden. Durch die enge Verzahnung mit dem Fachbereich Mathematik der Universität Kaiserslautern sowie durch zahlreiche Kooperationen mit internationalen Institutionen und Hochschulen in den Bereichen Ausbildung und Forschung ist ein großes Potenzial für Forschungsberichte vorhanden. In die Berichtreihe sollen sowohl hervorragende Diplom- und Projektarbeiten und Dissertationen als auch Forschungsberichte der Institutsmitarbeiter und Institutsgäste zu aktuellen Fragen der Techno- und Wirtschaftsmathematik aufgenommen werden.

Darüberhinaus bietet die Reihe ein Forum für die Berichterstattung über die zahlreichen Kooperationsprojekte des Instituts mit Partnern aus Industrie und Wirtschaft.

Berichterstattung heißt hier Dokumentation darüber, wie aktuelle Ergebnisse aus mathematischer Forschungs- und Entwicklungsarbeit in industrielle Anwendungen und Softwareprodukte transferiert werden, und wie umgekehrt Probleme der Praxis neue interessante mathematische Fragestellungen generieren.

Prof. Dr. Dieter Prätzel-Wolters
Institutsleiter

Kaiserslautern, im Juni 2001

Mathematics as a Technology: Challenges for the next 10 Years

Helmut Neunzert
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No doubt: Mathematics has become a technology in its own right, maybe even a key technology. Technology may be defined as the application of science to the problems of commerce and industry. And science? Science maybe defined as developing, testing and improving models for the prediction of system behavior; the language used to describe these models is mathematics and mathematics provides methods to evaluate these models. Here we are! Why has mathematics become a technology only recently? Since it got a tool, a tool to evaluate complex, "near to reality" models: Computer! The model may be quite old – Navier-Stokes equations describe flow behavior rather well, but to solve these equations for realistic geometry and higher Reynolds numbers with sufficient precision is even for powerful parallel computing a real challenge. Make the models as simple as possible, as complex as necessary – and then evaluate them with the help of efficient and reliable algorithms: These are genuine mathematical tasks.

Science is designed to "understand" natural phenomena, scientific technology extends the domain of validity of scientific theories to not yet existing systems. We create a new, virtual world, in which we may change and optimize much easier and quicker then in the real world. Even that is rather old – some scholars of ancient science (see for example Lucio Russo, The forgotten Revolution, Springer 2004) and some philosophers (see for example Max Scheler, Soziologie des Wissens, in "Die Wissensformen und die Gesellschaft", Francke-Verlag,1960) consider this interplay of science and technology as crucial for the birth of science during the Hellenistic period around 300 BC (with names like Euclid or Archimedes on top). But now, since we may mathematically optimize very complex virtual systems, we are able to use mathematics in order to design better machines, to minimize the risk of financial actions, to plan optimal surgery.

This is the reason why mathematics has become a key technology. The following technology fields emerged as crucial from several investigations in Europe (see A. Cliffe, B. Mattheij, H. Neunzert, (editors): MACSI-net Roadmap for Mathematics in European Industry, 2004, and H. Neunzert, U. Trottenberg (editors) "Mathematik als Technologie. Die Fraunhofer-Institute ITWM und SCAI", to appear):

- Simulation of Processes and Products
- Optimization, Control and Design
- Uncertainty and Risk
- Management and Exploitation of Data
- Virtual Material Design
- Biotechnology; Food and Health.

With help of these roadmaps which contain examples and challenges for future mathematics gathered from all over Europe, European mathematicians shall try to influence national and international research policies in a way that mathematics get the weight in future programs which it has in reality already now. Mathematics was too long in an ivory tower, often used only as brain exercises for students – it needs some time and a lot of effort to catch public awareness of its new role.

In this paper I shall show examples from different technology fields mentioned above, examples gained from our experience in the Fraunhofer Institute ITWM at Kaiserslautern. It was founded in 1996 and became a member of the Fraunhofer-Gesellschaft in 2001; the Fraunhofer-Gesellschaft is the leading German association for applied research with altogether 12.000 employees in ca. 60 institutes, an annual turnover of ca. 1.2 billion EURO and with branches in the US and in some European countries. Its decisive feature is, that basic funding is given proportional to what is earned in industry; to make a rather complicated story simple: A Fraunhofer Institute gets 40 cents from the federal government for each EURO it earns in industry. "No industrial project – no money at all" and "40 % on top in order to do fundamental research related to projects" these are the two rules which in my opinion are unique and uniquely successful worldwide.

ITWM has proved that mathematics as a technology is strong enough to follow the Fraunhofer rules. Not only that: At present it is the most successful institute of all the 15 Fraunhofer Institutes dealing with information technologies. The reason is: It has a huge market, much wider than any computer science institute. The disadvantage: the market doesn't yet know it. The consequence: There is a lot of space for all other really applied mathematicians and for cooperation. Worldwide!

But now I want to become more substantial. Here are the technology themes with examples and challenges (besides MACSI roadmap and the ITWM/SCAI paper see Fraunhofer ITWM, Annual Report 2003 (info@itwm.fraunhofer.de)).

Simulation of Processes and the Behavior of Products

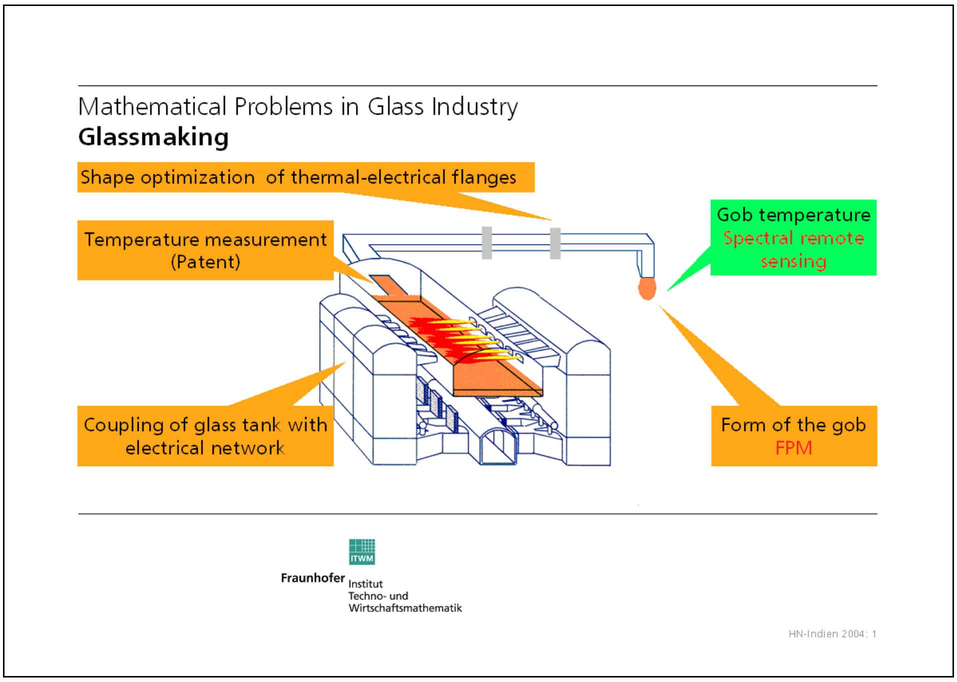
Simulation means: Modeling – computing – visualizing. To find the right model for the behavior of car components, as simple as possible and as complicated as necessary, is for example a task for asymptotic analysis: Identify small parameters in very complex models, study the behavior for these parameters tending to zero, estimating the error using this "parameter = 0 – model": All that is tricky perturbation theory, sometimes advanced functional analysis. But we should never "oversimplify" in order to get an analytically treatable model; very often numerics will be necessary – and very often advanced numerical ideas are necessary. Since a realistic geometry is sometimes very complex (think of a porous medium in a microscopic view) we need for example new, gridfree algorithms, efficiently implemented for parallel systems. And finally, long lists of numbers as a result of solving a PDE are completely useless – we have to interpret the results in terms of the original questions, quite often we have to visualize the results as images or movies.

Simulation is now routinely used in many parts of industry all over the world to support or to replace experimentation. "It can have a dramatic effect on the design process, reducing the need for costly prototypes and increasing the speed with which new products can be brought to market." (MACSI roadmap, page 9)

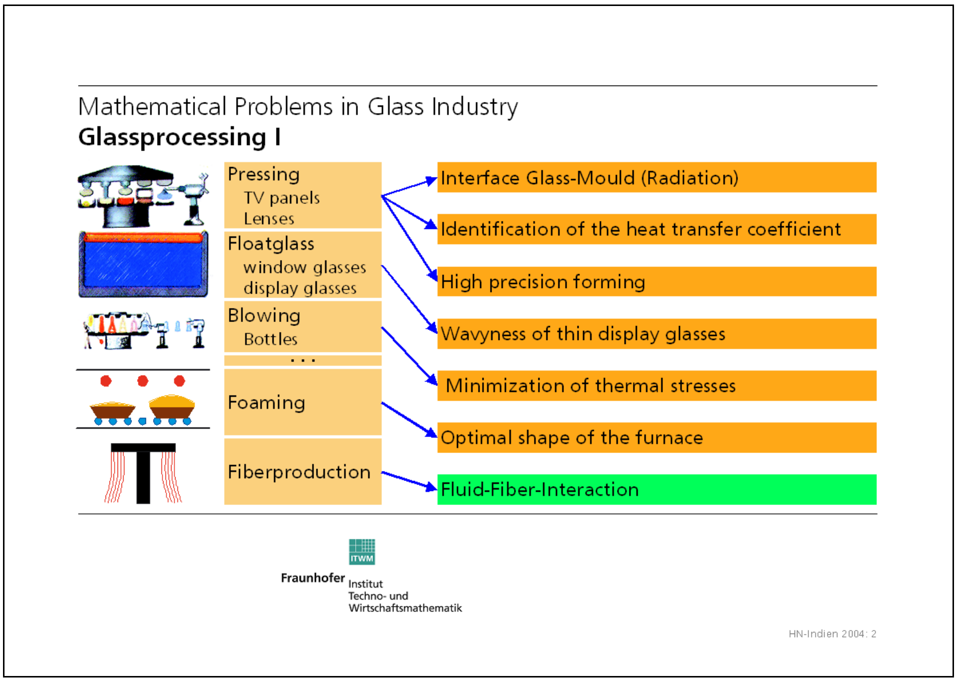
There are industries, where simulation has a long tradition, like aerospace or automotive industries or in oil and gas prospection. In these areas, commercial software is available and often easy to handle and efficient. It is (at least for a Fraunhofer institute) a very hard or even impossible task to place a new algorithm to substitute this kind of software – even if this algorithm is really better then the other one. What is possible for mathematicians is to substitute some modules in software products, as for example the second mathematical Fraunhofer institute SCAI does in offering an "Algebraic Multigrid Solver" for linear systems. Another possibility are post-processing algorithms enabling the user to do an "optimal experimental design" for virtual or (as A. A. Samarskij called it) "numerical experiments".

Industries operating with more basic technologies as textiles, glass or even metals just begin to use simulation. The market for commercial software seems too small and tailor made software is needed. How complicated this field could be will now be shown by our experience with glass industry. ITWM has a 10 year close cooperation with Schott Glas at Mainz, where cooperation may be taken literally: The enormous knowledge of Schott scientists about material and processes join mathematical ideas in ITWM to find innovative solutions. (The material was provided to me by Norbert Siedow from ITWM, some parts and literature are described in ITWM annual report 2003, page 26 ff)

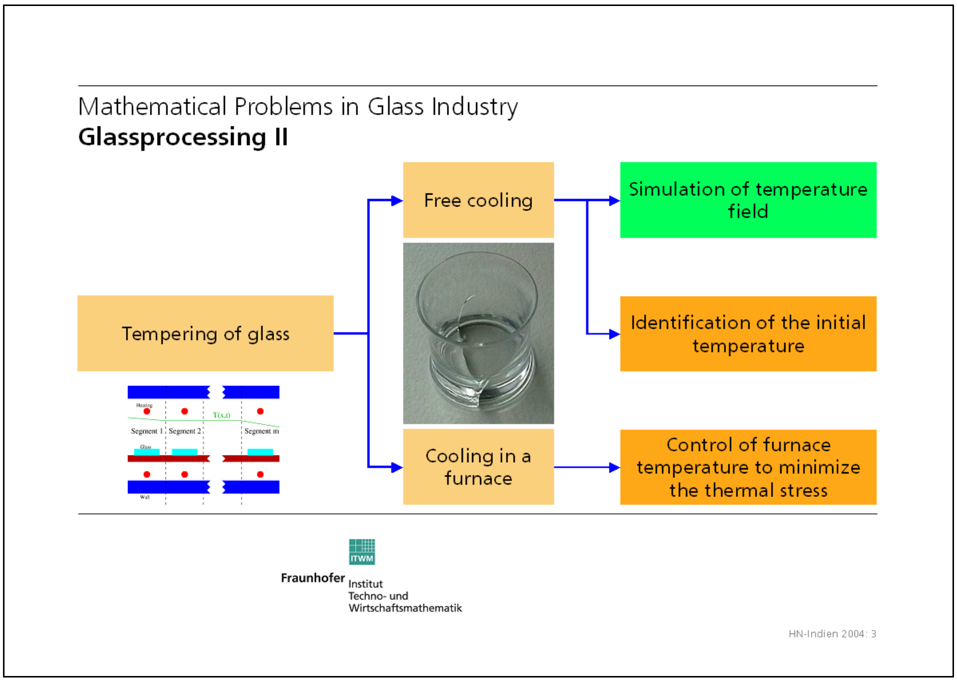
The first figure shows the glass making process, from the glass tank with molten glass of a temperature over 1000°C through a pipe to a kind of drop called gob; in this process we had identified 4 mathematical tasks which are denoted by colors. Two are so-called "inverse problems": To measure the temperature in the interior of the glass flow from radiation and to optimize the shape of the flanges carrying the pipe such that a given homogeneous temperature is created through electrical currents. The shape of the gob, a very viscous drop of liquid glass, has to be calculated by CFD codes able to handle free surfaces very well.



The next figures show different kinds of glass processing – and everywhere is mathematics: Pressing of TV panels ask for the simulation of radiation – in semi-transparent media a very elaborate task, since the radiation equation is a 6-dimensional integro-differential equation with enormous computational efforts.



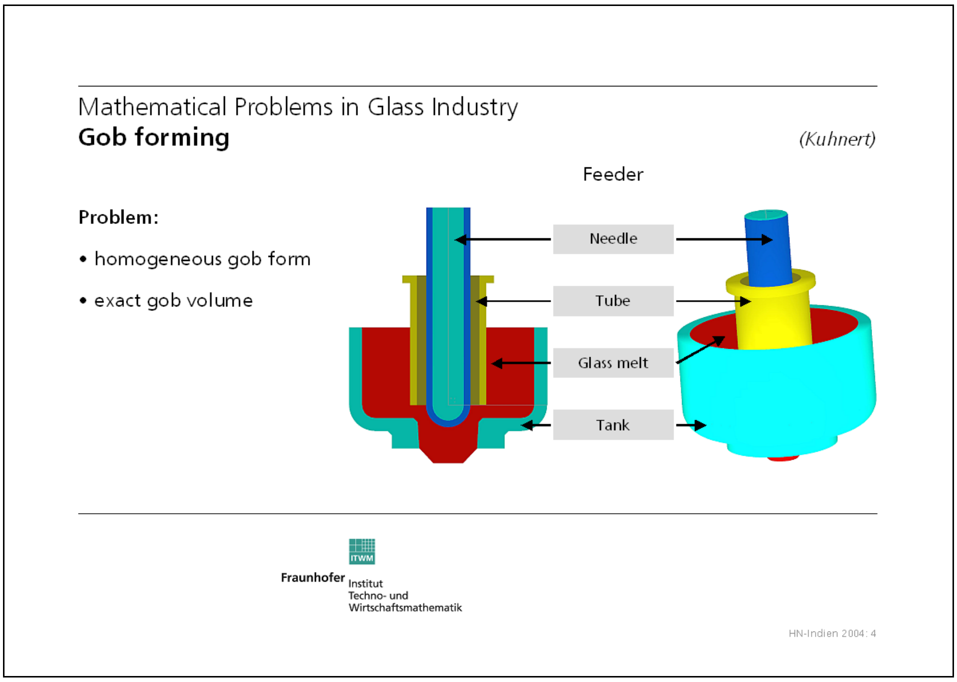
One uses tricky 2-scale asymptotics (see the PhD thesis of F. Zingsheim). Floatglass, an efficient production process invented by Pilkington, shows sometimes wavy patterns which have to be avoided. Whether these waves are instabilities created in a modification of the Orr-Sommerfeld equations is subject of an ongoing PhD-work. Glass fiber productions are extremely tricky processes in which the fibers interact with the air around them. Turbulent flow – fiber interaction is a topic, where turbulence models are not enough, but stochastic differential equations are crucial.



The last general figure 3 shows classical glass processing and problems connected with the cooling of glass. I would like to mention that already around 1800 Fraunhofer who gave the name to our society, produced lenses and had problems with the thermal tensions and the defects created by them.

Many of the problems here are "inverse problems", connected with heat transfer and they are very ill-posed. Inverse problems may be counted under "optimization" – it is the combination of optimization and simulation as in inverse problems, optimal shape design etc. which creates many mathematical challenges.

Let us have a closer look to a few of the problems. Figure 4 shows the details of gob forming.



The hot glass leaves the feeder, when the needle opens. A drop (gob) is formed and cut off by a special cutter. J. Kuhnert (ITWM) has designed a gridfree numerical method to calculate the glass flow – it is called "Finite Pointset Method" (FPM) and may be considered as an extension of "Smoothed Particle Hydrodynamics" (SPH). Particles are moving in the computational domain, carrying information about density, velocity, temperature etc. These information have to be extrapolated to other positions so that derivatives of these quantities as the Laplacian of the velocity components, the temperature gradient etc. can be calculated. These extrapolations are denoted by tilde – the rest is Lagrangean formalism.

Mathematical Problems in Glass Industry

Gob forming *(Kuhnert)*

Finite Pointset Method (FPM) – gridfree numerical method

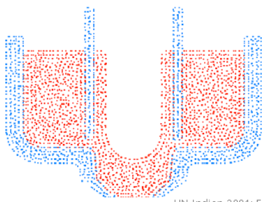
Movement of points $x_i^{n+1} = x_i^n + \Delta t \cdot v_i^n$

Pressure $0 = \nabla\left(\frac{1}{\rho}\nabla\left(p_{hyd}^{n+1}\right)\right); \ \tilde{p}_i^{n+1} = p_{hyd,i}^{n+1} + p_{dyn,i}^n$

Impulse equation $\frac{\tilde{v}_i^{n+1} - v_i^n}{\Delta t} = -\frac{1}{\rho}\nabla\left(\tilde{p}_i^{n+1}\right) + \frac{\eta}{\rho}\cdot\Delta\left(\tilde{v}_i^{n+1}\right) + g_i^{n+1}$

Energy equation $\frac{T_i^{n+1} - T_i^n}{\Delta t} = \frac{1}{\rho \cdot c}\nabla\left(k \cdot \nabla T_i^{n+1}\right)$

Correction of pressure and velocity $v^{n+1} \equiv \tilde{v}^{n+1} - \Delta t \frac{1}{\rho}\nabla\left(\varepsilon^{n+1}\right);$ $p_{dyn,i}^{n+1} = p_{dyn,i}^n - \varepsilon^{n+1}$



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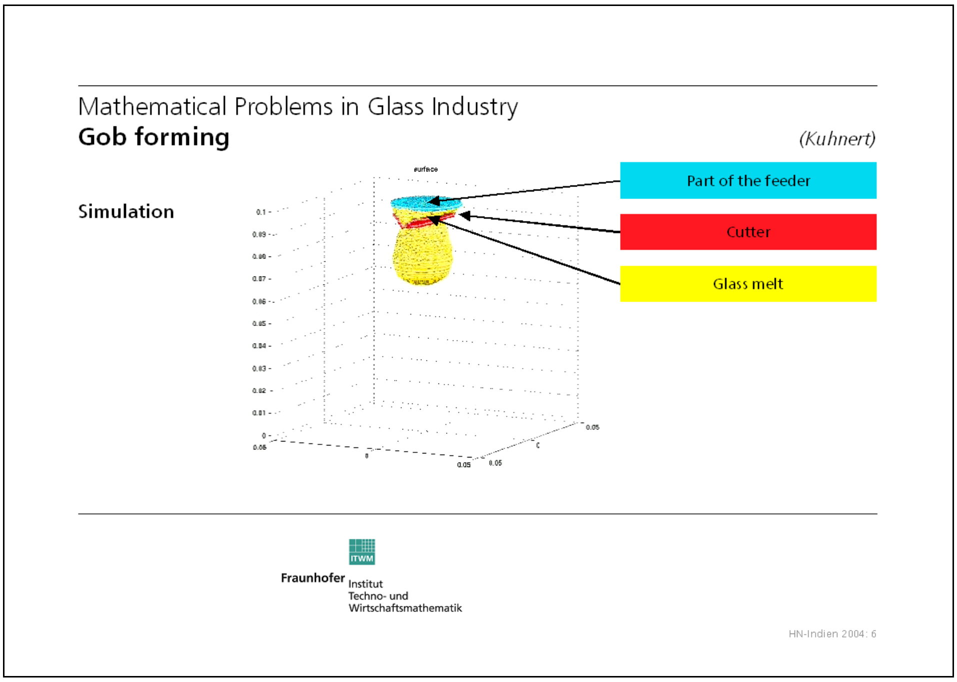
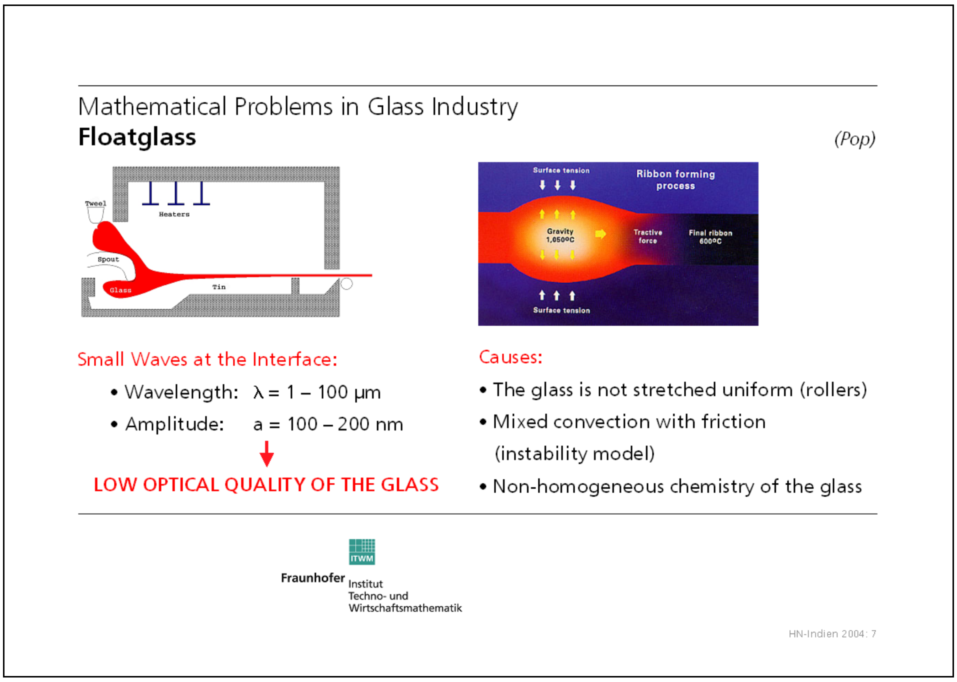
The method is appropriate for fluids with free boundaries, changing even the topology, as it happens, when the gob is cut off.

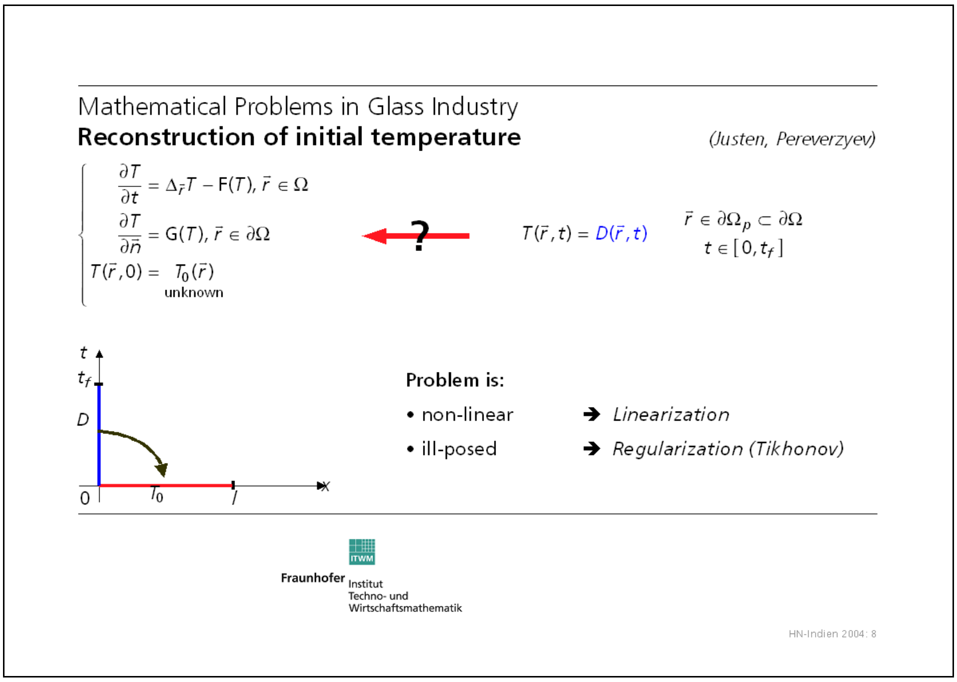


A more analytical task is the question of waves at floatglass surfaces. Here is the industrial question: What is the origin of waves at the interface of glass and molten tin (the glass flows over molten tin, a classical 2-phase flow with quite different temperatures) ? These waves are small defects which should be removed. What are the causes?



Let us finish the glass field by describing a very nice, very ill-posed problem which deals with temperature measurements. The high temperature of the glass melt asks for remote measurements or at least only measurements at the boundary.

Here is the problem:

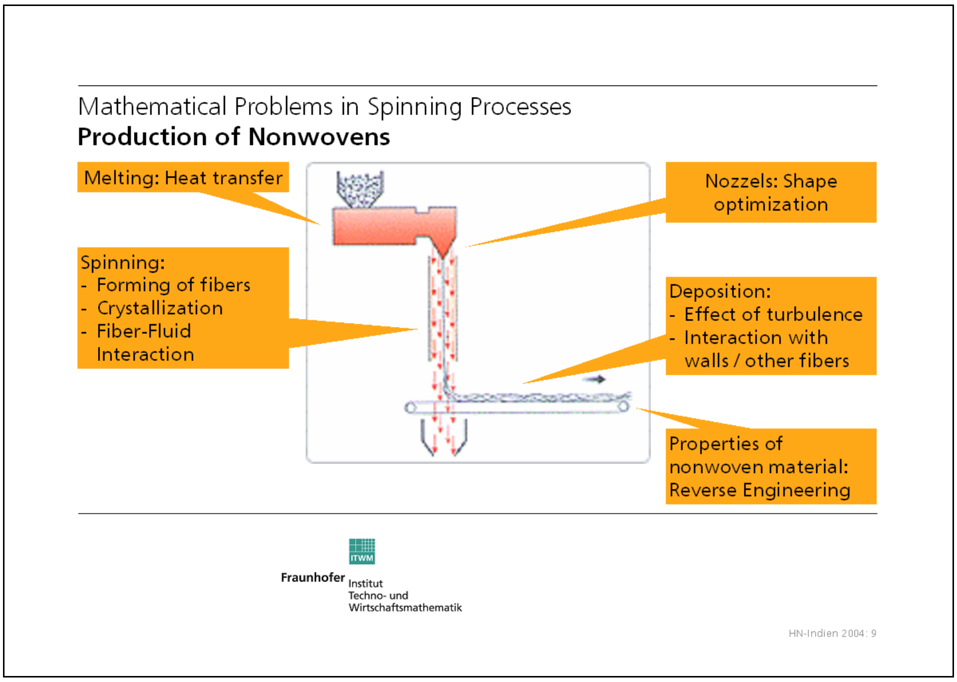


We measure the temperature at parts of the boundary; assuming that the heat transport is given by conduction and radiation and assuming the heat flux at the boundary is known everywhere – what is the temperature inside? If we would know the initial temperature, then… But we don't! Something "backward heat" should be in the problem.

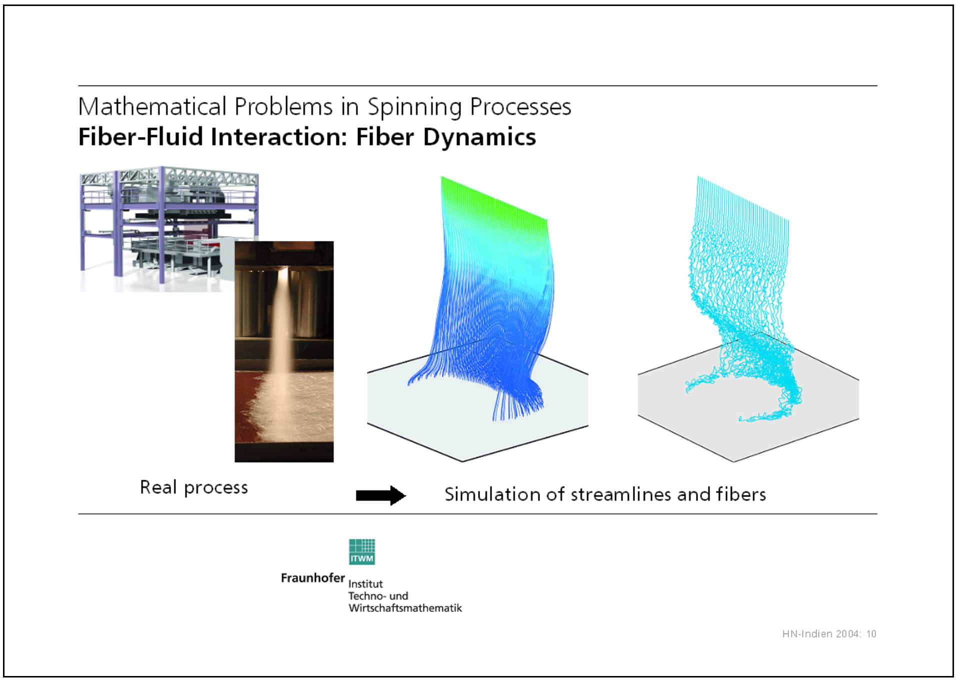
The problem was solved without radiation in a very nice master thesis by L. Justen and is with radiation subject of a PhD-thesis of Pereverzyev jun. For 1d it works, but real world is 3 d.

The situation is similar for melt spinning processes in textile industries; there is an intersection with the previous field, when we talk about glass fibers. But in general we have polymer fibers, leaving nozzles as a liquid, but crystallizing when an air flow is cooling and pulling the fibers.

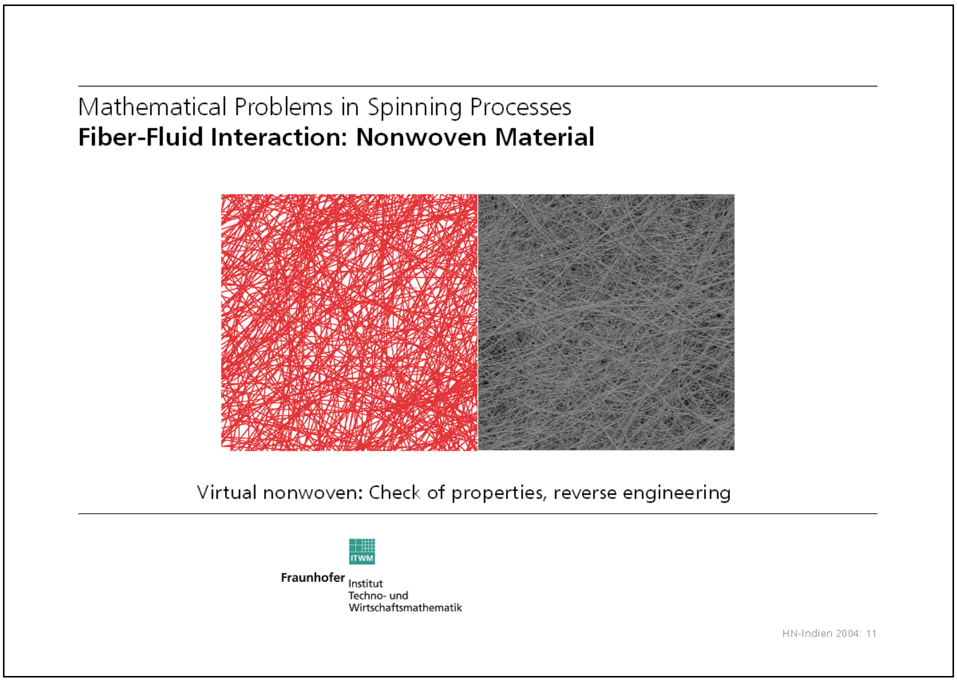
Here are some mathematical problems connected with the process:



Of course, there are curtains of fibers in a real process.



The industrial question belongs to “reverse engineering” : These are the properties of the product we want to have (even to describe these properties is a mathematical problem) – how can we create them?



The crystallization is a mathematical problem too and subject of a PhD-thesis of Renu Dhadwal . Let us have a closer look at the interaction of fibers with a turbulent flow. The main question is: How does the stochastic behavior of the turbulent air flow influence the (stochastically described) properties of the fabric. Here are some figures describing the work of N. Marheineke who just finished her PhD.

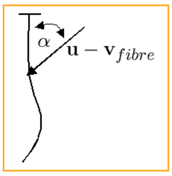
Mathematical Problems in Spinning Processes
Turbulence Effects

(Marheineke)

Asymptotic 1D-Model of fiber dynamic:

$$\rho A \partial_{tt}\mathbf{r}(s,t) = \partial_s[T(s,t)\partial_s \mathbf{r}(s,t)] - EI\partial_{ssss}\mathbf{r}(s,t) + \rho A \mathbf{g} + \mathbf{f}^{air}(s,t),$$

$$(\partial_s \mathbf{r})^2(s,t) = 1 \qquad \text{+ boundary conditions}$$



Force due to turbulent flow:

$$\mathbf{f}^{air}(s,t) = \mathbf{f}^{air}(\mathbf{u}(\mathbf{r}(s,t),t)) \quad \text{with} \quad \|\mathbf{f}^{air}\| = \frac{1}{2}\rho^{air}\, d\, \|\mathbf{u} - \mathbf{v}_{fibre}\|^2 C_\alpha$$

Turbulence-Model (k-ϵ based on RANS Equations)

$$\mathbf{u}(\mathbf{x},t) = \bar{\mathbf{u}}(\mathbf{x},t) + \mathbf{u}'(\mathbf{x},t) \Rightarrow \bar{\mathbf{u}},\ k,\ \epsilon$$

Idea: Force-Model ➔

$$\mathbf{f}^{air}(\bar{\mathbf{u}} + \mathbf{u}') \approx \underbrace{\mathbf{f}^{air}(\bar{\mathbf{u}})}_{deterministic\ \bar{\mathbf{f}}} + \underbrace{\frac{d\mathbf{f}^{air}}{d\mathbf{u}}\Big|_{\mathbf{u}=\bar{\mathbf{u}}}\mathbf{u}'}_{stochastic\ \mathbf{f}'}$$

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Mathematical Problems in Spinning Processes
Turbulence Effects

(Marheineke)

Direct Numerical Simulation (DNS)

♯ grid points ~ $\mathrm{Re}^{9/4}$

- enormous computat. effort
- restricted to simple applicat.

↓

Large Eddy Simulation (LES)

direct simulation of large vortices

stochastic approximation of small vortices effect

- high computational effort
- use for improving / verifying stochastic models

Stochastic Models for RANS

$$\mathbf{u}(\mathbf{x},t) = \bar{\mathbf{u}}(\mathbf{x},t) + \mathbf{u}'(\mathbf{x},t)$$

$$\nabla \cdot \bar{\mathbf{u}} = 0$$

$$\partial_t \bar{\mathbf{u}} + (\bar{\mathbf{u}} \cdot \nabla)\bar{\mathbf{u}} = -\frac{\nabla \bar{p}}{\rho} + \nabla \cdot (2\nu \bar{\mathbf{S}} - \overline{\mathbf{u}'\mathbf{u}'^T})$$

Reynolds–stress tensor

Stress Transport Models

6 additional transport eqs.

- high demands on numerics
- hardly use in practise

0-, 1-, 2-Eq Models

Boussinesq eddy viscosity:

$$-\overline{\mathbf{u}'\mathbf{u}'^T} = 2\nu_T \bar{\mathbf{S}} - \frac{2}{3}k\mathbf{I}$$

ν_T: turbulent viscosity

k: turbulent kinetic energy

- closure conditions

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Mathematical Problems in Spinning Processes

Turbulence Effects *(Marheineke)*

k-ϵ Model

Turbulent kinetic energy

$$k = \tfrac{1}{2}\overline{\mathbf{u}' \cdot \mathbf{u}'}$$

Dissipation rate

$$\epsilon = \nu\, \overline{\nabla \mathbf{u}' : \nabla \mathbf{u}'}$$

Determination by means of transport equations with additional closure conditions

$$\partial_t k + \underbrace{\bar{\mathbf{u}} \cdot \nabla k}_{Conv_k} = \underbrace{-\overline{\mathbf{u}'\mathbf{u}'^T} : \nabla \bar{\mathbf{u}}}_{Prod_k} \underbrace{-\nu \overline{\nabla \mathbf{u}' : \nabla \mathbf{u}'}}_{Diss_k} \underbrace{+\nabla \cdot \left[\nu \nabla k - \frac{1}{2}\overline{(\mathbf{u}' \cdot \mathbf{u}')\mathbf{u}'} - \frac{\overline{p'\mathbf{u}'}}{\rho}\right]}_{Diff_k}$$

Dimensional ↓ analysis

Characteristic turbulent scales: $v_T = k^{1/2}, \quad l_T = k^{3/2}/\epsilon, \quad t_T = k/\epsilon$

➔ Turbulent viscosity $\nu_T = C\, v_T\, l_T = C\, k^2/\epsilon$

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Mathematical Problems in Spinning Processes

Turbulence Effects *(Marheineke)*

Assumption: locally homogeneous, isotropic, frozen turbulence

Construct random Gaussian field for velocity fluctuations $(\mathbf{u}'_{(\mathbf{x},t)}, \mathbf{x} \in \mathbb{R}^3, t \in \mathbb{R}_0^+)$

$$\mathbf{u}'(\mathbf{x}, t) = \mathbf{u}'(\mathbf{x} - \bar{\mathbf{u}}t, 0) = \mathbf{u}'(\mathbf{x} - \bar{\mathbf{u}}t)$$

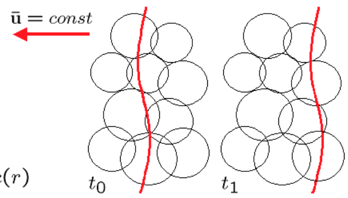
with

mean $\mathbb{E}[\mathbf{u}'_\mathbf{x}] = 0$

covariance / correlation tensor

$$\mathbb{E}[\mathbf{u}'(\mathbf{x}) \otimes \mathbf{u}'(\mathbf{x} + \mathbf{r})] = \Gamma(\mathbf{r})$$

$\Gamma(\mathbf{r})$ can be expressed by 1D correlation function $c(r)$



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Mathematical Problems in Spinning Processes

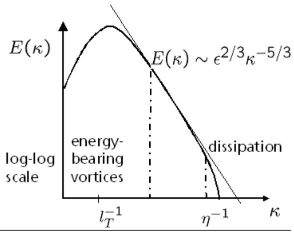
Turbulence Effects *(Marheineke)*

Choose $c(r) := 2\int_0^\infty E(\kappa)\frac{\sin(\kappa r) - \cos(\kappa r)\kappa r}{\kappa^3 r^3}\, d\kappa$ with $E(\kappa) \in \mathcal{C}^2(\mathbb{R}_0^+)$

+ further demands

Then $(\mathbf{u}'_{(\mathbf{x},t)}, \mathbf{x} \in \mathbb{R}^3, t \in \mathbb{R}_0^+)$ is differentiable and satisfies:

- Kolmogorovs energy spectrum
- $\overline{\mathbf{u}' \cdot \mathbf{u}'} = 2k$
- $\overline{\nabla \mathbf{u}' : \nabla \mathbf{u}'} = \epsilon/\nu$



Integrated Gaussian field for stochastic force along the fiber

Asymptotic: $\mathbf{f}'(s,t)$ white noise in space and time

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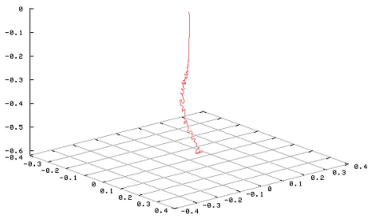
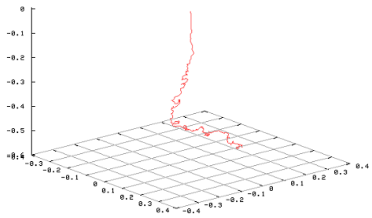
Mathematical Problems in Spinning Processes

Turbulence Effects *(Marheineke)*





Fiber dynamics

without stochastic force | with stochastic force

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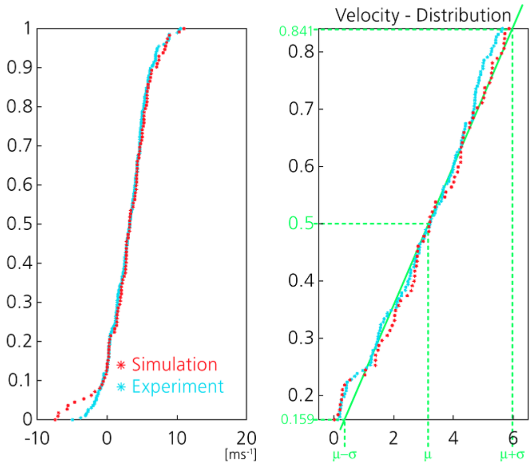
Mathematical Problems in Spinning Processes

Turbulence Effects *(Marheineke)*

Statistic evaluation of simulations with measurements:

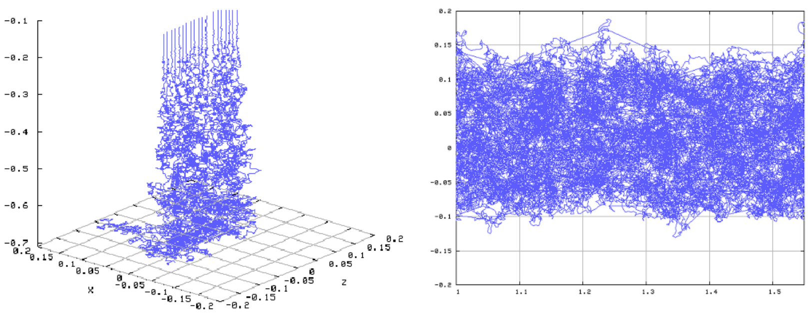
- same probabilty function for fiber velocity components → normal distribution
- small difference of standard deviation → $|\sigma_{Exp} - \sigma_{Sim}|/\sigma_{Exp} < 0.1$

→ good conformity



Mathematical Problems in Spinning Processes

Deposition with Turbulence Effects



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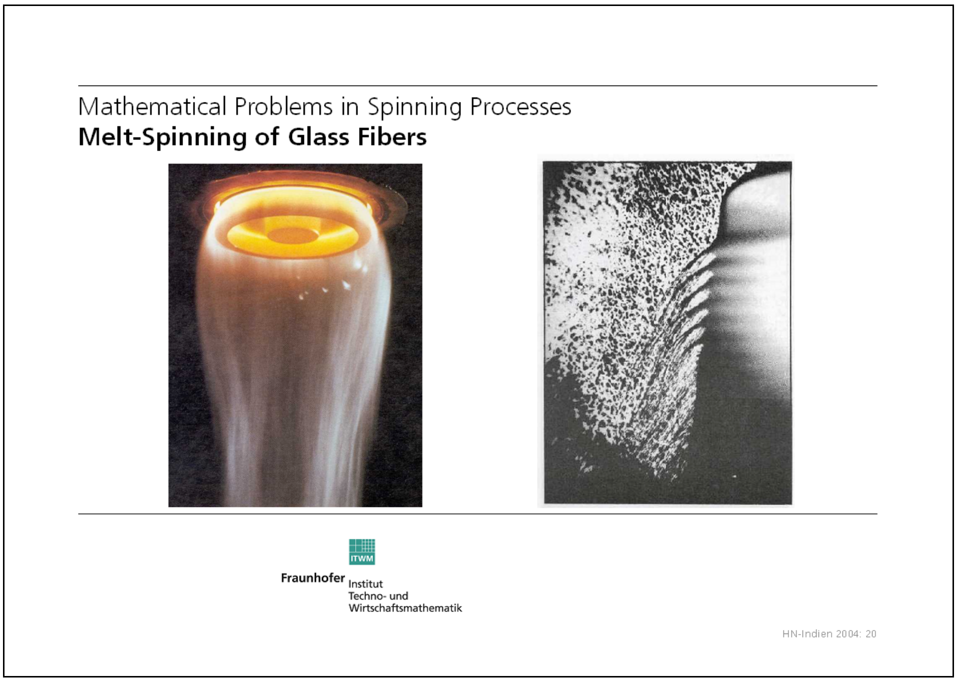
Things may even be more complicated – see for example a quickly rotating spinneret for producing glass fibers:



Optimization, Control and Design

What we finally want to achieve in our man-made world are optimal solutions, the process should be as cheap, as fast as possible, the product should at least behave better then the products of the competitors. (Even nature seems to have a creator who is interested in optimality – that is why we have so many variational principles; and that is why animals and plants show us so many tricky solutions for their "technical" problems to be as stable, as light, as smoothly moving as possible and necessary. This is called "bionics" – and there may be an interesting interplay between optimization by mathematics and optimization by evolution) "So rather then asking how a product performs, the question is, how should the product be designed in order to perform in a specified way. … Scheduling, planning and logistics also fall within that area of optimization. Optimal control is used to provide real-time control of an industrial process or a product, such as a plane or a car, in response to current operating conditions. A related area is that of inverse problems, where the parameters (or even the structure) of a model must be estimated from measurement of the system output." (MACSI roadmap, page 13)

We have mentioned inverse problems already in (1); they appear literally everywhere. We will show 2 examples from our projects at ITWM, however very short.

There is the wide field of topological shape optimization; "topological" means, that one may change the topology of a structure for example by admitting holes. One has to minimize an objective function (maximal stress, mean compliance) etc. with respect to the shape.

Topological optimization

Given a domain Ω and corresponding to it, the problem of linear elasticity in Ω:

$$-div\ \sigma(u_\Omega) = \rho f \quad \text{in } \Omega; \text{ where}$$

u_Ω denotes the displacements in Ω, $\sigma(u_\Omega)$ the corresponding stresses, linear depending on the strains

$$e(u_\Omega) = \left(\frac{1}{2}\left(\frac{\partial u_{\Omega_j}}{\partial x_i} + \frac{\partial u_{\Omega_i}}{\partial x_j}\right)\right), \quad \sigma = Ae.$$

The boundary conditions are:

$$\sigma(u_\Omega)n = t,\ t \text{ given surface on a part of } \partial\Omega$$

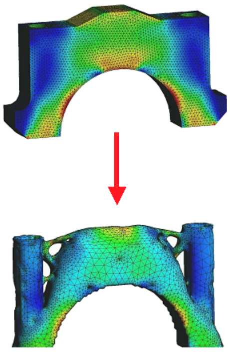
$$u_\Omega = 0 \text{ at the rest of } \partial\Omega, \text{ where the body is damped.}$$

We want to change Ω, such that a functional

$$\Omega \longrightarrow \mathbf{J}(\Omega, u_\Omega) = j(\Omega)$$

is minimal. This functional may be the mean compliance

$$\Omega \longrightarrow \mathbf{J}(\Omega, u_\Omega) = \int_\Omega Ae(u_\Omega) \cdot e(u_\Omega) dx$$



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Mathematical ideas

(a) Characterize Ω by level set of functions φ

$$\Omega = \{x : \varphi(x) < 0\},\ \partial\Omega = \{x : \varphi(x) = 0\}$$

$$\Omega \leftrightarrow \varphi,\ u_\Omega = u_\varphi$$

(b) Use the concept of topological gradient: Drill a hole in Ω of radius ρ at point $x \in \Omega$:

$$\Omega_\rho^{(x)} = \Omega / \kappa_\rho(x)$$

and study, how **J** changes by that operations for small ρ

$$\lim_{\rho \to 0} \frac{j(\Omega_\rho(x)) - j(\Omega)}{\lambda(\rho)} = g(x) = \text{topological gradient.}$$

$\lambda(\rho)$ depends on **J**, but is often proportional to the volume of the hole.

$g(x) < 0 \Rightarrow$ **J** is improved by drilly a small hole at x.

The more negative g is, the more more you gain. $\Rightarrow$ Reduce the domain at points, where g is minimal.

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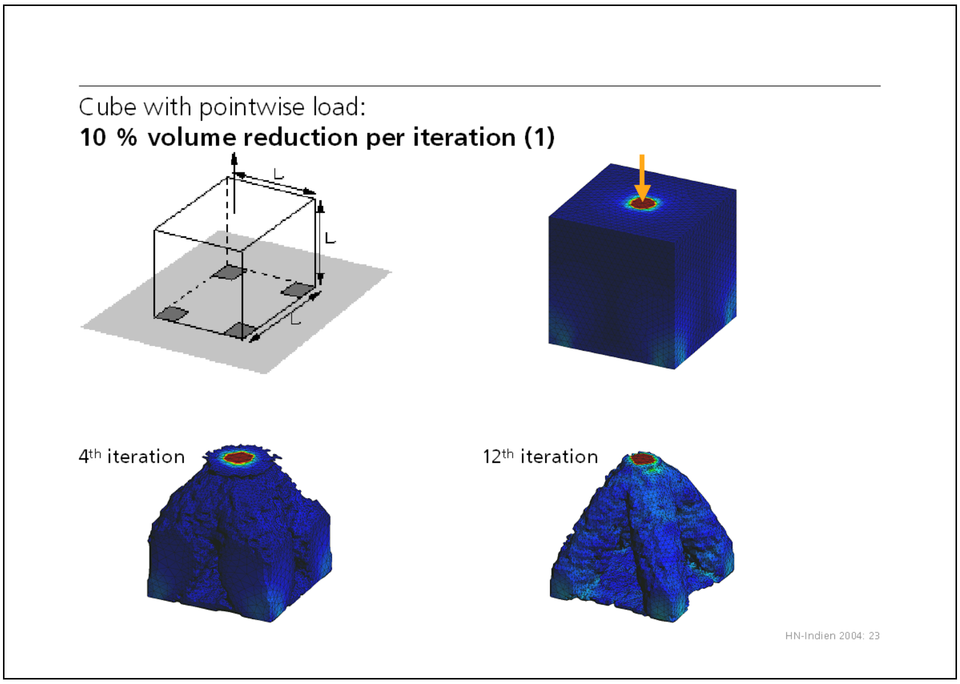
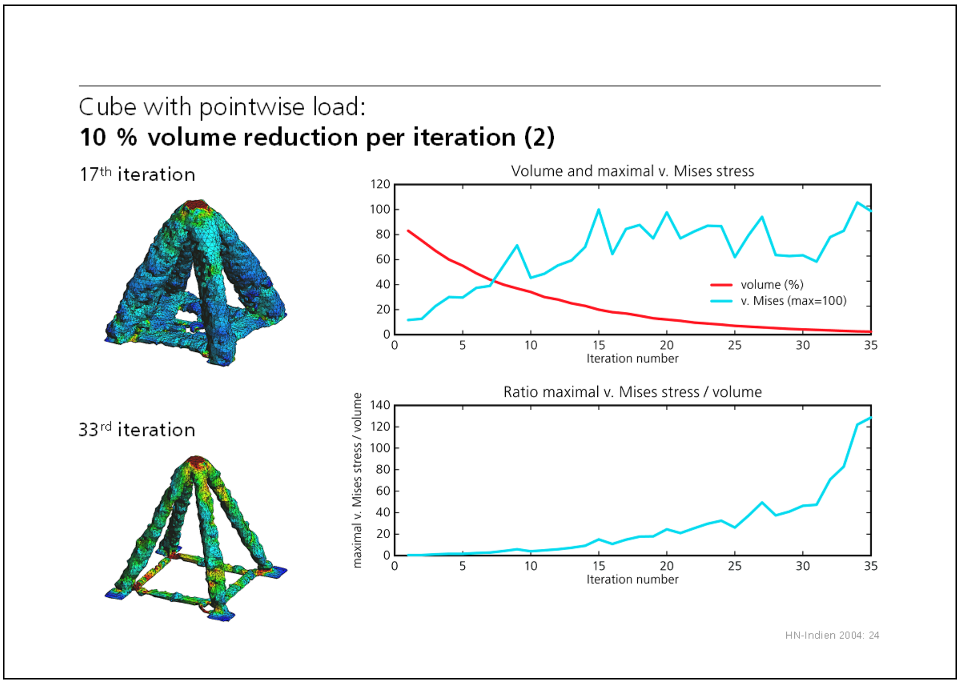
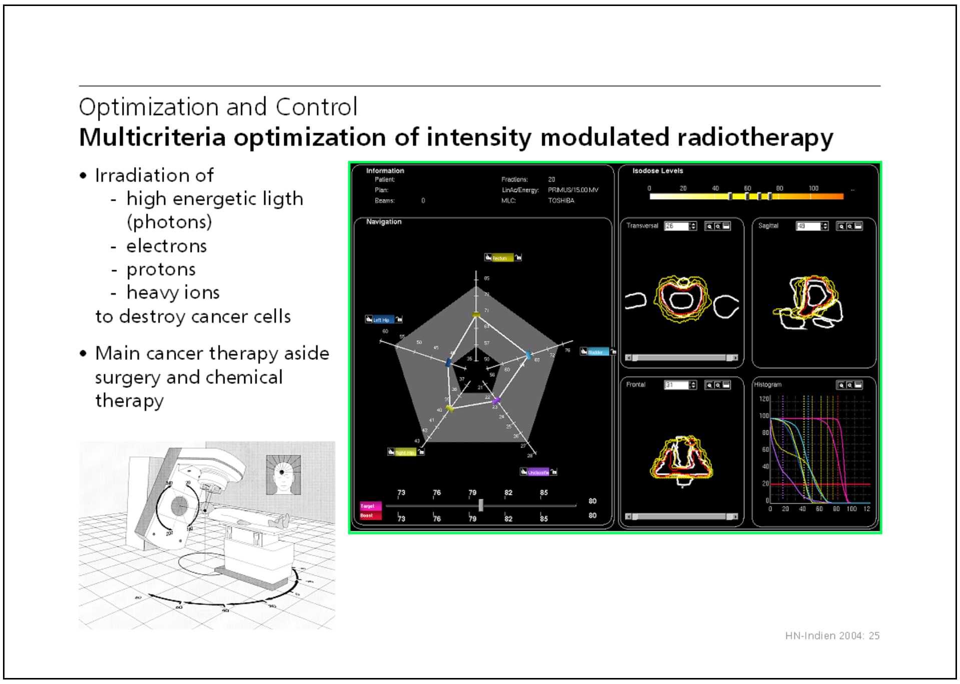


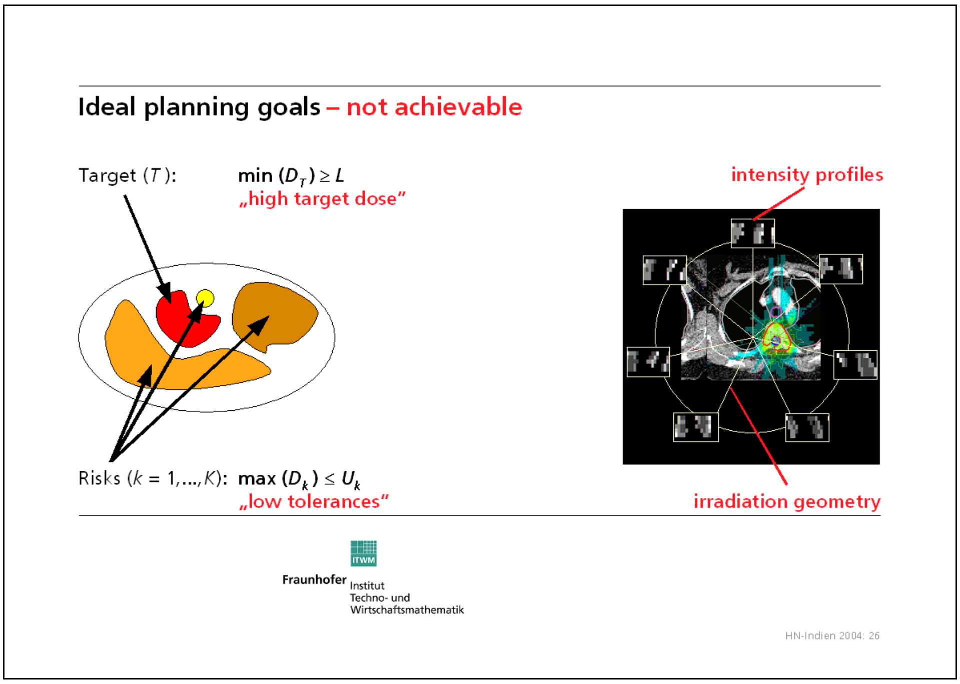


As an example for a multicriteria optimization we consider a project of ITWM together with Harvard medical school and Siemens:

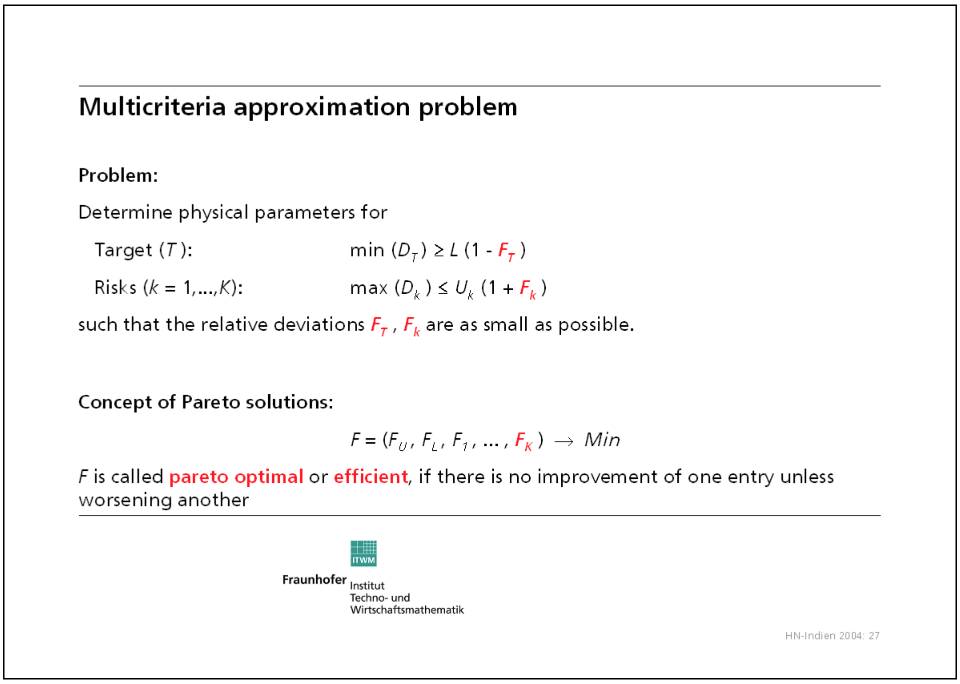
How should we optimally control the radiation in cancer therapy such that the cancer cells are destroyed as much as possible but at the same time organs or important healthy parts of the body remain undamaged. There are, besides optimization, a lot of simulation problems, f. e. to simulate how radiation penetrates the body; but let's concentrate on optimization assuming that the transmission of the radiation to different parts of the body given the external source, which can be controlled, is known. The goal is, that a medical doctor can operate with the optimization tool, allowing more or less radiation to certain organs by "pulling" in the corresponding direction of a navigation scheme; the program then computes the different doses of different sources and different directions, getting at the end corresponding isodose levels.



To be more detailed: we have a target, the tumor and we have "risks", which should get as little as possible, but at most at given thresholds for the radiation.



One uses Pareto solutions, which are defined in the next figure:



To do this so fast, that it is finally online, and to do it so, that the doctors can easily handle it, are interesting and highly relevant mathematical tasks.

Uncertainty and Risk

Many processes in nature, in economy and even in daily life are or seem to be strongly accidental; we therefore need a stochastic theory in order to model these processes. Randomness creates uncertainty, uncertainty creates risk, for example in decisions about investments, about medication, about security of technical systems like planes or power plants.

Whether this randomness is genuine or just a consequence of high complexity is a philosophical question which does not influence stochastic modeling. Very complex systems you will find in catastrophes like earthquakes or floods; extremely complex are biological systems, for example the human body. Experiments are not possible, simulation is therefore highly necessary, but very difficult, too.

Also in economy experiments are impossible, but one needs help for decisions which minimize the risk.

The law of large numbers leads often to models which are deterministic PDEs and very similar to deterministic models in natural sciences. But at a closer look they are even more complex, for example very high dimensional (the independent variables are not geometric, but maybe the values of different stocks). Therefore even if we get at the end a treatable PDE, we have to use Monte-Carlo methods to solve them approximately – and we are back to stochastic differential equations. Now quite often derivatives of these solutions with respect to variables and parameters are needed – and to differentiate a function given by a Monte-Carlo method is not always successful. Here the Malliavin calculus, initially not invented for practical problems, is a great help (see for example Fournier et al: Application of Malliavin calculus to Monte-Carlo methods in finance, Finance and Stochastics 3 (4) 1999). Here an example from option prizing:

Malliavin calculus for Monte-Carlo methods (1)

Let $\Phi(t,x)$ be the price of an option at time t, where x is the present price of stocks underlying the option. Then

$$\frac{\partial \Phi}{\partial(t)} + \langle b, \nabla\Phi \rangle + \frac{1}{2}\sigma\sigma^T \Delta\Phi = 0,$$

where the final payoff of the option, $\Phi(T,x)$ is given by $f(x)$.

A Monte-Carlo method computes Φ by

$$\Phi(t,x) = E(f(X(T)/X(t) = x)$$

as an expectation value, where $X(t)$ is a solution of

$$dX(\tau) = b(X(\tau))d\tau + \sigma(X(\tau))dW(\tau).$$

f interest is often $\nabla_x\Phi(t,x)$, called **"delta"**.

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Malliavin calculus for Monte-Carlo methods (2)

To compute delta, we use the "Malliavin calculus".

If Ω is a space of paths ("Wiener space") and

$F : \Omega \to \mathbb{R}$ (in 1d) is a random variable, one defines a "directional derivative"

$$D_\gamma F(\omega) := \frac{d}{d\varepsilon} F(\omega + \varepsilon\gamma)/\varepsilon = 0\ ,$$

$$\text{where } \gamma = \gamma(t) = \int_0^t g(s)ds, \qquad g \in \mathbb{L}^2.$$

If F possesses derivatives in all possible directions γ and if there exists an $\Psi(t,w)$ such that

$$D_0 F(\omega) = \int_0^T \Psi(t,w)g(t)dt$$

then F is called "differentiable" and $\mathbb{D}_t F(\omega) := \Psi(t,w)$

Malliavin calculus for Monte-Carlo methods (3)

There is an "integration by parts" formula, which leads to

$$\nabla u(x) = E\left(f(X(T)\frac{1}{T}\int_0^T \sigma^{-1}(\, X(t)Y(t)\,)^* \, dW(t) \Big/ X(0) = x \right);$$

here $u(x) = \Phi(0, X)$ and Y is the "linearization around X"

$$dY(\tau) = b'(X(\tau)Y(\tau) + \sum_{i=1}^{n} \sigma_i'(X(\tau))Y(\tau)dW_i(\tau) \;\; ; \;\; Y(0) = E_n$$

Realize, that $\frac{1}{T}\int_0^T \sigma^{-1}(\, X(t)Y(t)\,)^* \, d(W(T)$ doesn't depend on f.

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Malliavin calculus for Monte-Carlo methods (4)

A European option with one stock underlying

$$dP(t) = P(t)[\, rdt + \sigma dW(t)\,], \quad P(0) = p$$

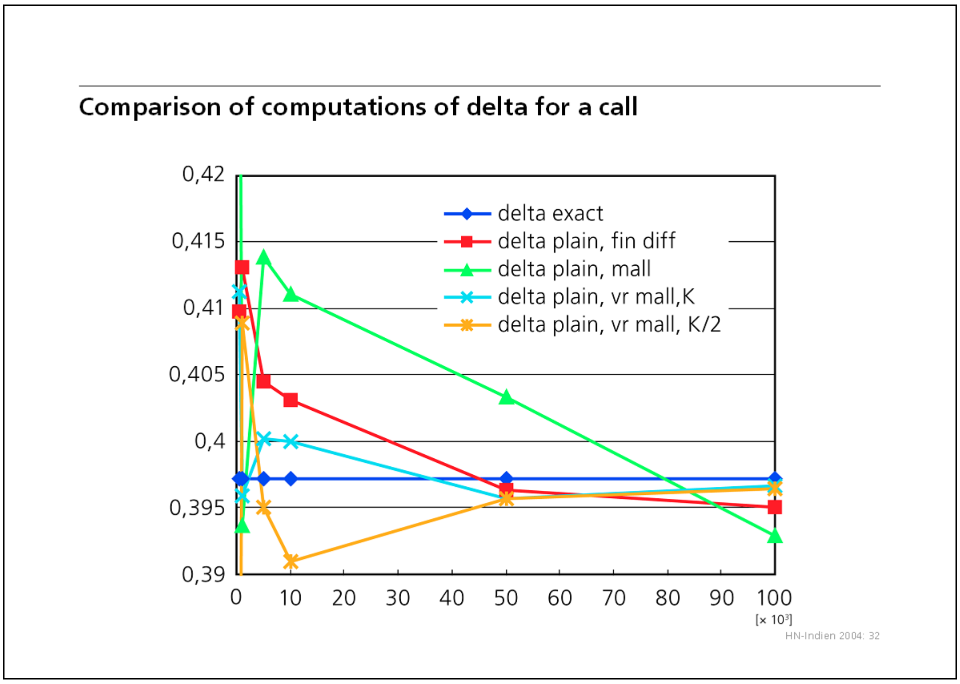
We call $\tilde{u}(p) = E\left(e^{-rT} f(P(T)\right)$ the **option prize;**

then $$\tilde{u}'(p) = e^{-rT} E\left(f(P(T)) \cdot \frac{W(T)}{p\sigma T} \right)$$

This expactation value is simple to compute by simulation,

since again $\frac{W(T)}{p\sigma T}$ is independent of f.

However, for example for $f(x) = (x - K)_+$, the variance is very high and one needs many runs. If we do variance reduction methods, we get the following picture.

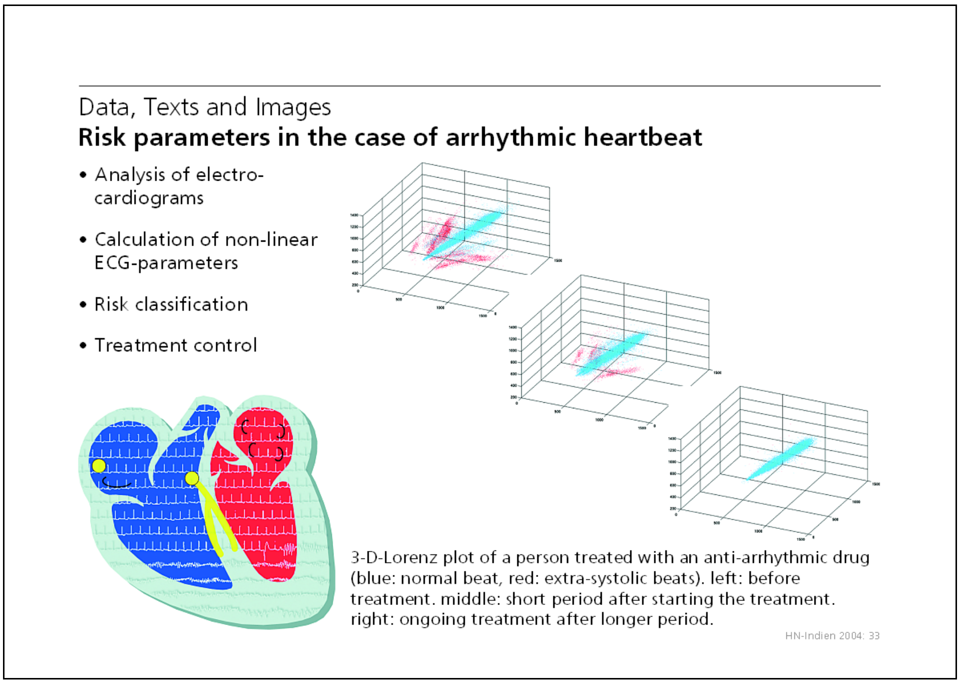


Of course there are other uncertainties and risks – in floods, earthquakes. In technical systems, very different methods are involved.

Management and Exploitation of Data

We are flooded by data which, if structured, create information and finally knowledge. To extract this information or knowledge from data is called "data mining". Data may be given as signals or images; if we want to discover patterns, if we want to "understand" these signals or images, we need image processing and pattern recognition methods. If we want to study and predict input-output systems for which we do not have enough theory (simple models) but many observations from the past, we may develop "black-box" models like linear control models or neural networks. If for parts of the system a theory is available, we may talk of "grey-box" models. Data mining, signal or image processing and black or grey-box models are the mathematical disciplines involved here. Some of them are not as mature as PDE, optimization or stochastics, but certainly a field, where new ideas are needed. (There are many, especially in the field of pattern recognition: look for example at articles of David Munford or Yves Meyer from the last 10 years.)

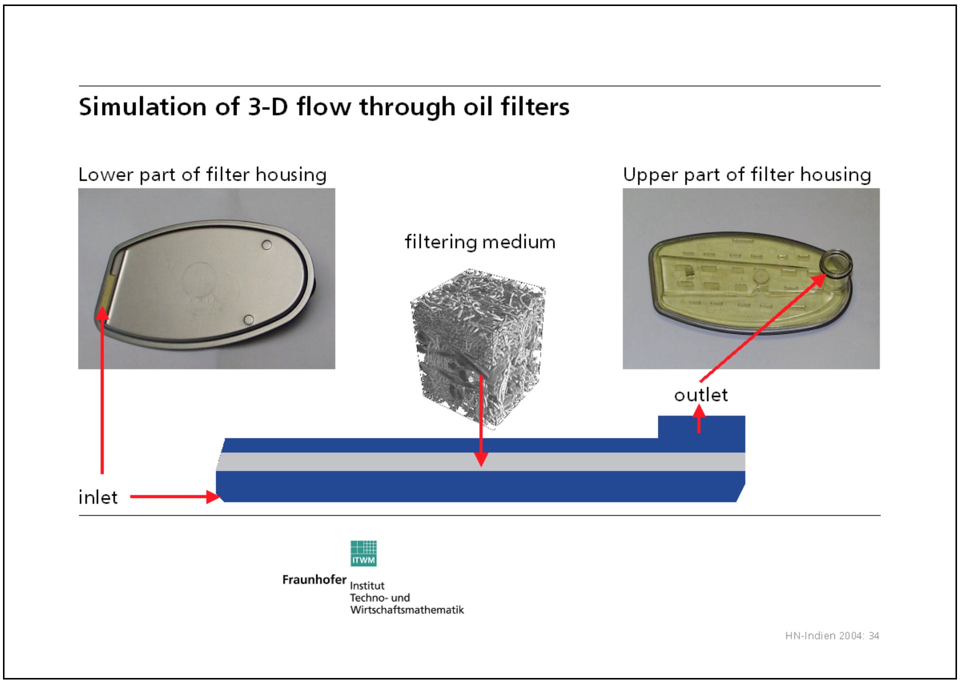
A typical input-output system, where we do not have much theory, is the human body; medicine is therefore a main application area and we want to show only one example from our experience, the interpretation of long term electrocardiograms. If we register only the heart beats, we get quite long sequences $(t_i)_{i=1,\dots N}$ with N~100 000 and have to find the information about the risk for sudden cardiac death. To do so we use Lorenz plots, sets consisting of points $\{(t_i, t_{i+1}, t_{i+2}), (t_{i+1}, t_{i+2}, t_{i+3}), \dots\}_{i=1,\dots N}$ and try to understand the structure of these sets. Of course the beat is rather regular, if the Lorenz plot is a slim club (but too slim is again dangerous). The picture shows the clearly visible influence of drugs; to estimate the risk one needs very tricky data mining techniques.

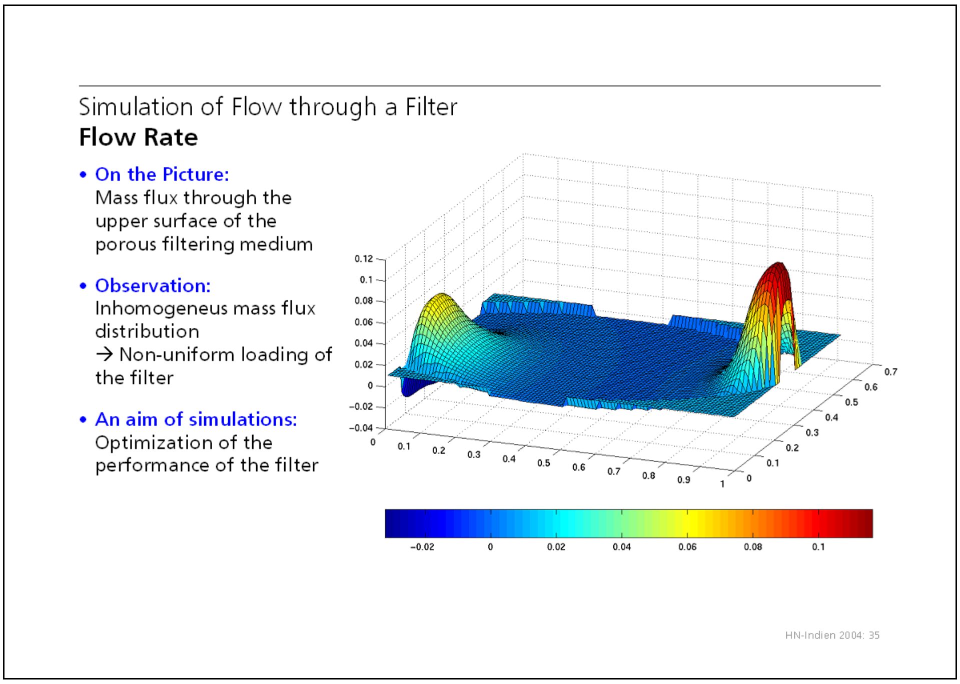


Virtual Material Design

One of the objectives of material science is to design new materials which have desirable properties; to do so by using simulation is called "virtual material design". Mathematics is used to relate the large-scale (macroscopic) properties of materials such as stiffness, fatigue, permeability, impedance to the small-scale (microscopic) structure of the material. The microscopic structure has to be optimized in order to guarantee the required macroscopic properties. This is an application of multi-scale analysis, where we use averaging and homogenization procedures to pass from micro to macro. The scales may reach from nano to the size of constituents of composite materials. Typical materials are textiles, paper, food, drugs, alloys.

At ITWM we try to design appropriate filter material; this is a very wide field, since filters are used everywhere – they serve different purposes and require therefore different properties. The example deals with oil filters – the research work is in its first part done by Iliev and Laptev from ITWM.





We use a system which we get through homogenization from Navier-Stokes through a “very porous ” medium- a Navier-Stokes-Brinkman system which is a combination of incompressible, steady Navier-Stokes with a Darcy term.

Simulation of 3-D flow through oil filters

Model:

Incompressible laminar flow through filters.
Navier-Stokes-Brinkman type system in whole domain (justification Angot 1998):

$$\begin{cases} \underbrace{-\nabla\cdot(\tilde{\mu}\nabla\bar{u}) + (\rho\bar{u},\nabla)\bar{u}}_{\text{Navier-Stokes}} + \overbrace{\frac{\mu}{\tilde{K}}\bar{u} + \nabla p}^{\text{Darcy's law}} = \bar{f} \\ \nabla\cdot\bar{u} = 0 \end{cases}$$

momentum equations

continuity equation

$$[\bar{u}]|_{\Gamma} = 0;$$
$$[\bar{n}\cdot(\tilde{\mu}\nabla u - pI)]|_{\Gamma} = 0.$$

Interface conditions are already incorporated

$$\tilde{K}^{-1} = \begin{cases} K^{-1}, & \bar{x}\in\Omega_{por} \\ 0, & \bar{x}\in\Omega_{liq} \end{cases}$$

Fictitious Regions Method – type continuation of coefficients

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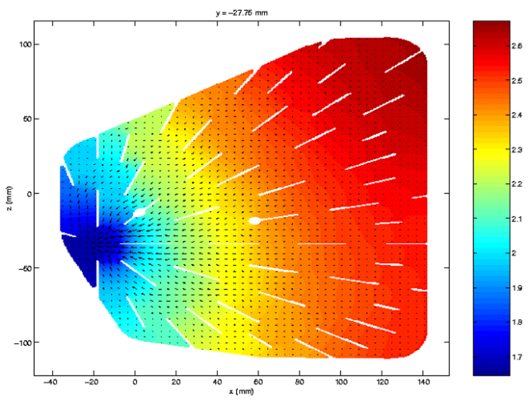
The interface condition describing the behavior of the fluid on the surface of the filter material is a rather delicate issue, but in this model (with Brinkman homogenization) easier to handle (see the PhD-thesis by Laptev). The flow field is given in the following:

Simulation of 3-D flow through oil filters

Pressure (colors) and velocity field (arrows) in a cross-section of an oil filter



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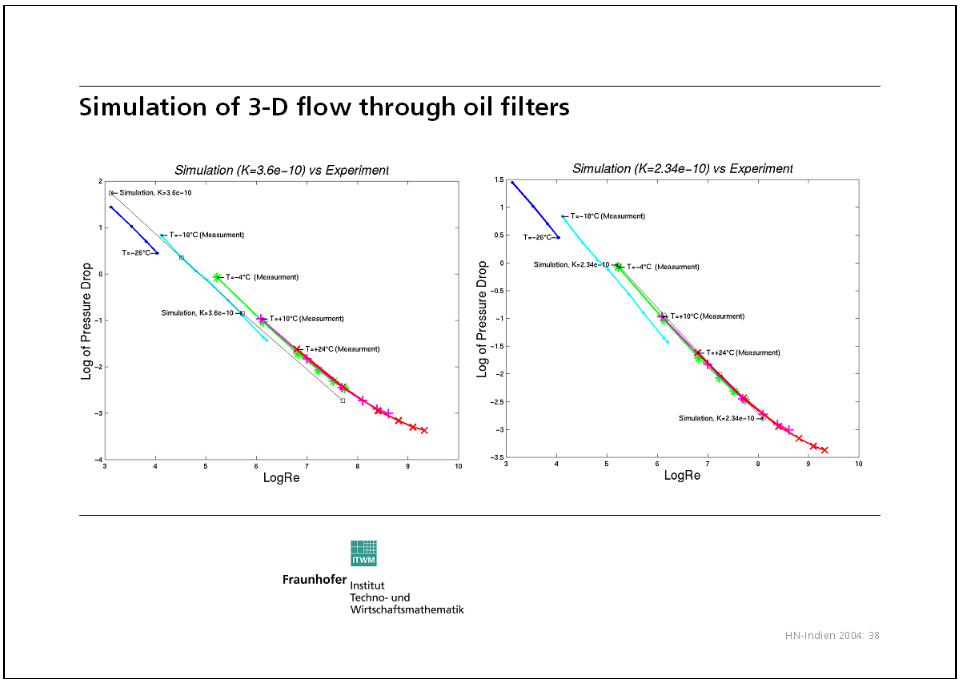
The correspondence with measurements (where the pressure loss for different Reynold numbers at different temperatures with correspondingly different permeabilities) is remarkable.



I call this correspondence sometimes "prestabilized harmony" – a rather crude model which is numerically approximated, gives results which correspond with nature to an extent which one really might not expect. But, of course, care is necessary – models have their range of applicability, their limitations should be carefully respected.

To compute the flow field of a filter is not enough to understand its efficiency; the transport of the particles, which have to be filtered out, must be simulated; therefore, we have to model their absorption by the fibers of the filter; the motion of the particles by the fluid velocity, its friction, the influence of diffusion; finally the absorption is, of course, filter and particle dependent. This is an area of exciting modeling (see for example some reprints by A. Latz from ITWM).

Biotechnology, Food and Health

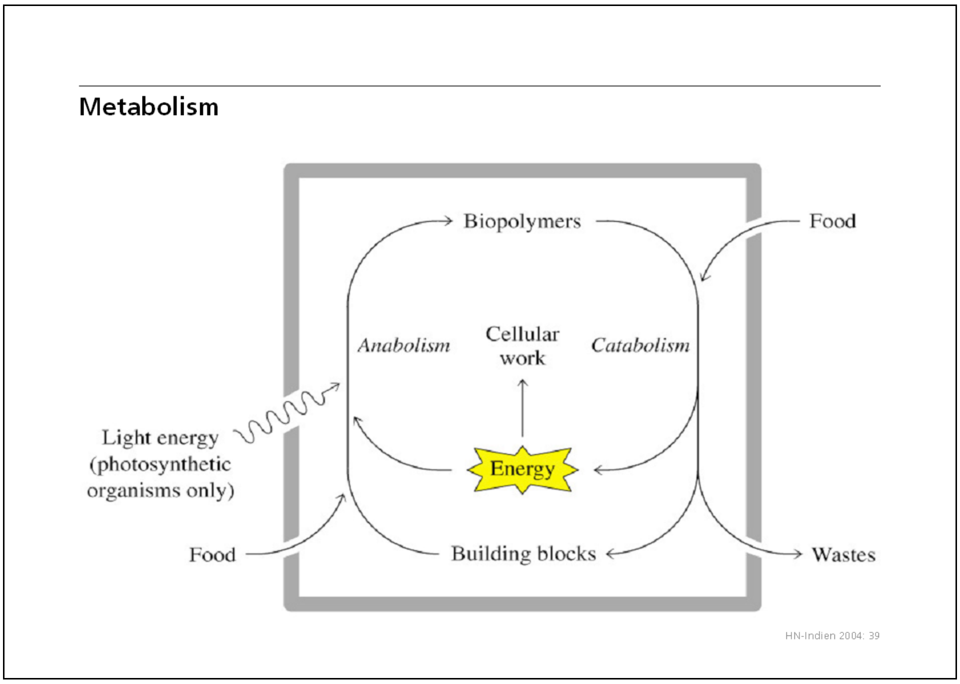
This field has created new research areas which are rather interdisciplinary – for example bioinformatics or system biology. Statistics, discrete mathematics, computer science and system and control theory, data mining, differential-algebraic systems, parameter and structure identification are involved, together with all kinds of life sciences. Biological systems are extremely complex, involving huge molecules which interact in poorly understood ways. It is a long way to get a full understanding in terms of fundamental chemistry and physics. And it is a mathematical task to gain as much information as possible from the data we have; the classical idea to use a linear control system and identify the coefficients does not work. We therefore need "grey models", complex enough to allow prediction, but simple enough that parameters may be identified from the measurements.

Health is very much related to deterministic models for biophysical processes, a better image understanding and efficient data mining.

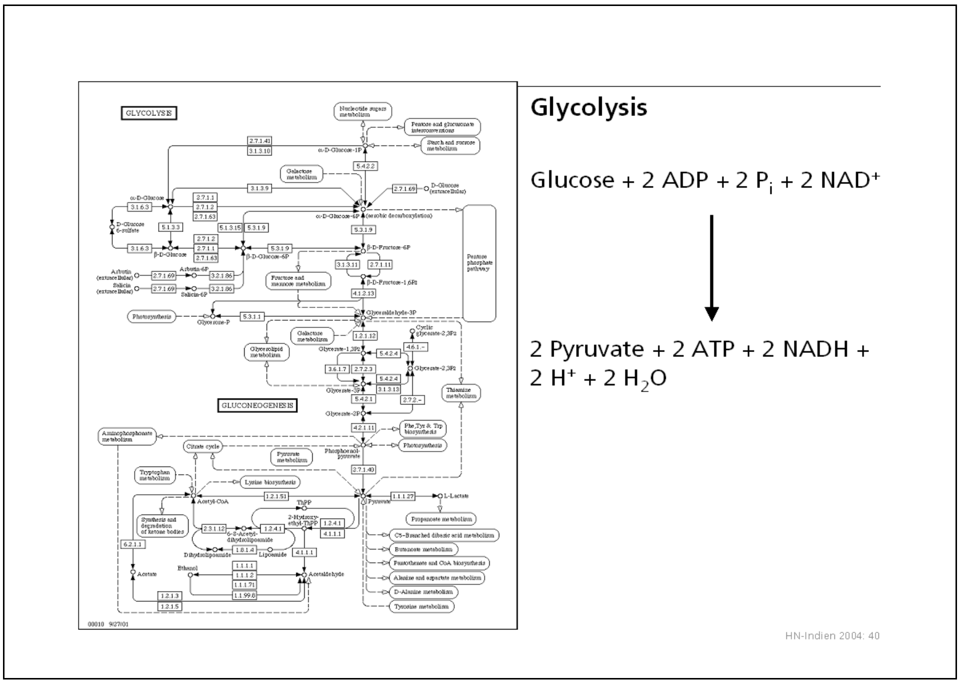
Food is one of the emerging application fields of science, especially simulation. To simulate a process preparing food, for example cooking of an omelette, frying a piece of meat in order to optimize the quality or the energy consumption, are mathematical tasks of extremely high difficulty. However, the economic value is enormous, for companies which offer food worldwide and for companies which produce for example household appliances.

The ITWM has not yet many projects in this field; however, its joint venture with Chalmers University of Technology, the Fraunhofer Chalmers Research Centre (FCC) at Gothenburg deals with bio-informatics and system biology. The figures are taken from a presentation by Mats Jirstrand, FCC.

By metabolism we mean the processes inside living cells.



These are complicated biochemical processes, even a "simple" process as glycolysis is not at all simple.

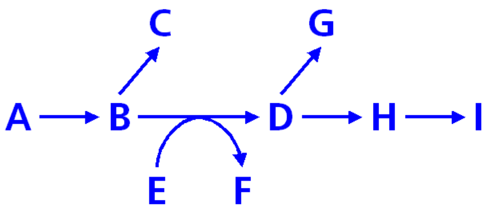


We have to model biochemical pathways, i. e. chains of reactions.

Modeling of Biochemical Reactions

Chemical Reactions: $A \longrightarrow B$ $\quad A + B \longleftrightarrow C \longrightarrow D$

Biochemical Pathways/ Networks (chains of reactions):



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Reactions happening in collisions change the concentration of molecules of different types.

Modeling of Biochemical Reactions

Reaction rate in $dV \cong$ number of collisions $\cong$
number of collisions per sek of reactants in $dV \cong$
probability, that n_a molecules of type A and n_b molecules of type B enter dV simultaneously (independent events)

$$p(A)\dots p(A)p(B)\dots p(B) = p(A)^{n_a}\, p(B)^{n_b} \cong [A]^{n_a}[B]^{n_b}$$

Hence, $r_{dV} = k_0\ [A]^{n_a}[B]^{n_b}$ (but k_0 is volume dependent)

Double volume $\Rightarrow$ double k_0

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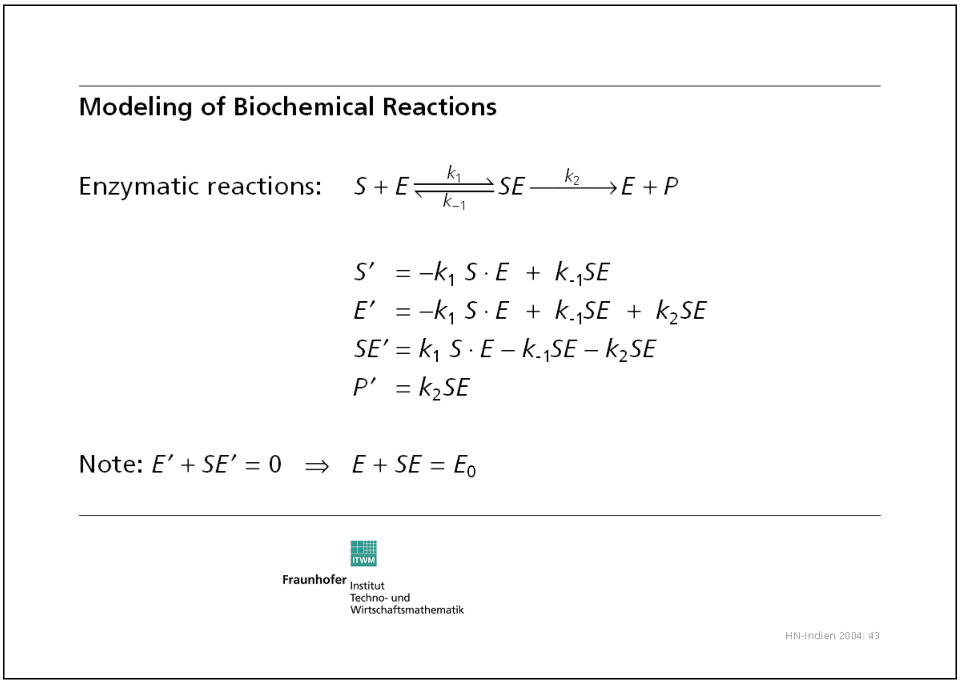
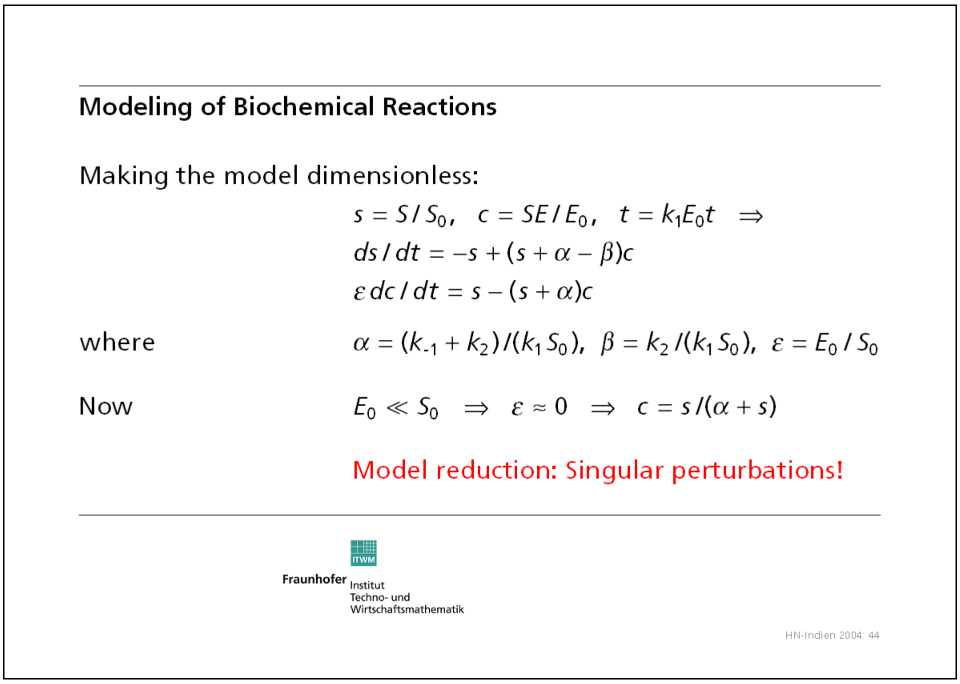
Even simple enzymatic reactions lead to non-linear systems.



Finally one does what every modeler has to do: We non-dimensionalize and look for small parameters to apply perturbation methods.



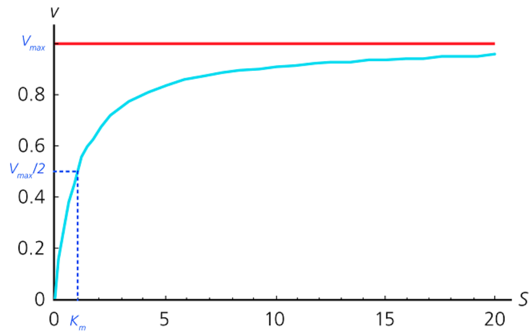
This leads to rational expression, called Michaelis-Menten dynamics in biology.

Modeling of Biochemical Reactions

$$ds/d\tau = -\beta s/(\alpha + s) \quad \Leftrightarrow$$

$$dS/dt = -V_{max} S/(K_m + S) \qquad \text{...Michaelis-Menten dynamics}$$

where $V_{max} = k_2 E_0, \quad K_m = (k_{-1} + k_2)/k_1$



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At the end we get very large, rational right hand sides for system of ODEs.

The problem is: We do not know the parameters of the system – even the structure (which reactions should be included, do we need to include hysteresis etc.) is not clear. Can we deduce from the behavior which structural elements the model should include? And how many parameters are we able to identify? How can we adopt the model to the knowledge we have? Some steps are done, but there is still a long way to go.

Conclusions

As mentioned in the beginning and shown during the description of the technology fields, one of the major drivers behind the dramatic change towards a knowledge-based economy is the advent of powerful and affordable digital computers. The rate of progress in hardware follows Moore's Law, telling us that computer power doubles every two years. Equally important, but not so widely appreciated, is the fact that there has been a similar improvement in the algorithms, used to evaluate complex mathematical models. The improvement in speed, due to better algorithms, has been as significant as the improvements in hardware. All this has made computer simulation an accepted tool, first in science: Computational X is dominating. Industry is already feeling the benefits of these advances, resulting in an increase in efficiency and competitiveness. This in turn makes mathematics, being at the core of all simulation, to become a key technology. Mathematics by its abstraction allows to transfer ideas from one application field to another. Mathematicians are "cross thinkers". This kind of cross thinking creates creativity and leads to innovation.

To give mathematics its power, the classical "engineering mathematics" is not sufficient. I hope I have made clear that new ideas, some from pure mathematics too, are needed in order to get good results: New function spaces, new ideas in non-linear analysis or in stochastic calculus, new ideas to deal with inverse problems, to deal with pattern recognition etc. etc. It is not a question of "pure or applied", there is a need for "pure and applied". Both should be in balance and they should work together; the fact that there is a wide-spread separation, weakens both parts.

There is a need for properly educated mathematicians all over the world, too. What a proper education means for an "industrial mathematician", would be a subject in its own. The European Consortium for Mathematics in Industry (ECMI) has put a lot of effort into that issue. However, what we have to strive after is creativity and flexibility in finding proper models and more efficient algorithms. "Industrial Mathematics" or, as it is called in Europe, Technomathematics, Economathematics or Finance Mathematics are not subjects in its own like algebra or topology, it is more a new attitude towards the world, it is the curiosity in order to understand and the drive to improve.

If we mathematicians work together, if we are courageous enough to leave the ivory tower of our science and act in the real world, I am sure we shall see a bright future for our science, and for our students, too.

Published reports of the Fraunhofer ITWM

The PDF-files of the following reports are available under:
www.itwm.fraunhofer.de/de/zentral__berichte/berichte

1. D. Hietel, K. Steiner, J. Struckmeier

A Finite - Volume Particle Method for Compressible Flows

We derive a new class of particle methods for conservation laws, which are based on numerical flux functions to model the interactions between moving particles. The derivation is similar to that of classical Finite-Volume methods; except that the fixed grid structure in the Finite-Volume method is substituted by so-called mass packets of particles. We give some numerical results on a shock wave solution for Burgers equation as well as the well-known one-dimensional shock tube problem.
(19 pages, 1998)

2. M. Feldmann, S. Seibold

Damage Diagnosis of Rotors: Application of Hilbert Transform and Multi-Hypothesis Testing

In this paper, a combined approach to damage diagnosis of rotors is proposed. The intention is to employ signal-based as well as model-based procedures for an improved detection of size and location of the damage. In a first step, Hilbert transform signal processing techniques allow for a computation of the signal envelope and the instantaneous frequency, so that various types of non-linearities due to a damage may be identified and classified based on measured response data. In a second step, a multi-hypothesis bank of Kalman Filters is employed for the detection of the size and location of the damage based on the information of the type of damage provided by the results of the Hilbert transform.
Keywords: Hilbert transform, damage diagnosis, Kalman filtering, non-linear dynamics
(23 pages, 1998)

3. Y. Ben-Haim, S. Seibold

Robust Reliability of Diagnostic Multi-Hypothesis Algorithms: Application to Rotating Machinery

Damage diagnosis based on a bank of Kalman filters, each one conditioned on a specific hypothesized system condition, is a well recognized and powerful diagnostic tool. This multi-hypothesis approach can be applied to a wide range of damage conditions. In this paper, we will focus on the diagnosis of cracks in rotating machinery. The question we address is: how to optimize the multi-hypothesis algorithm with respect to the uncertainty of the spatial form and location of cracks and their resulting dynamic effects. First, we formulate a measure of the reliability of the diagnostic algorithm, and then we discuss modifications of the diagnostic algorithm for the maximization of the reliability. The reliability of a diagnostic algorithm is measured by the amount of uncertainty consistent with no-failure of the diagnosis. Uncertainty is quantitatively represented with convex models.
Keywords: Robust reliability, convex models, Kalman filtering, multi-hypothesis diagnosis, rotating machinery, crack diagnosis
(24 pages, 1998)

4. F.-Th. Lentes, N. Siedow

Three-dimensional Radiative Heat Transfer in Glass Cooling Processes

For the numerical simulation of 3D radiative heat transfer in glasses and glass melts, practically applicable mathematical methods are needed to handle such problems optimal using workstation class computers. Since the exact solution would require super-computer capabilities we concentrate on approximate solutions with a high degree of accuracy. The following approaches are studied: 3D diffusion approximations and 3D ray-tracing methods.
(23 pages, 1998)

5. A. Klar, R. Wegener

A hierarchy of models for multilane vehicular traffic
Part I: Modeling

In the present paper multilane models for vehicular traffic are considered. A microscopic multilane model based on reaction thresholds is developed. Based on this model an Enskog like kinetic model is developed. In particular, care is taken to incorporate the correlations between the vehicles. From the kinetic model a fluid dynamic model is derived. The macroscopic coefficients are deduced from the underlying kinetic model. Numerical simulations are presented for all three levels of description in [10]. Moreover, a comparison of the results is given there.
(23 pages, 1998)

Part II: Numerical and stochastic investigations

In this paper the work presented in [6] is continued. The present paper contains detailed numerical investigations of the models developed there. A numerical method to treat the kinetic equations obtained in [6] are presented and results of the simulations are shown. Moreover, the stochastic correlation model used in [6] is described and investigated in more detail.
(17 pages, 1998)

6. A. Klar, N. Siedow

Boundary Layers and Domain Decomposition for Radiative Heat Transfer and Diffusion Equations: Applications to Glass Manufacturing Processes

In this paper domain decomposition methods for radiative transfer problems including conductive heat transfer are treated. The paper focuses on semi-transparent materials, like glass, and the associated conditions at the interface between the materials. Using asymptotic analysis we derive conditions for the coupling of the radiative transfer equations and a diffusion approximation. Several test cases are treated and a problem appearing in glass manufacturing processes is computed. The results clearly show the advantages of a domain decomposition approach. Accuracy equivalent to the solution of the global radiative transfer solution is achieved, whereas computation time is strongly reduced.
(24 pages, 1998)

7. I. Choquet

Heterogeneous catalysis modelling and numerical simulation in rarified gas flows
Part I: Coverage locally at equilibrium

A new approach is proposed to model and simulate numerically heterogeneous catalysis in rarefied gas flows. It is developed to satisfy all together the following points:
1) describe the gas phase at the microscopic scale, as required in rarefied flows,
2) describe the wall at the macroscopic scale, to avoid prohibitive computational costs and consider not only crystalline but also amorphous surfaces,
3) reproduce on average macroscopic laws correlated with experimental results and
4) derive analytic models in a systematic and exact way. The problem is stated in the general framework of a non static flow in the vicinity of a catalytic and non porous surface (without aging). It is shown that the exact and systematic resolution method based on the Laplace transform, introduced previously by the author to model collisions in the gas phase, can be extended to the present problem. The proposed approach is applied to the modelling of the EleyRideal and LangmuirHinshelwood recombinations, assuming that the coverage is locally at equilibrium. The models are developed considering one atomic species and extended to the general case of several atomic species. Numerical calculations show that the models derived in this way reproduce with accuracy behaviors observed experimentally.
(24 pages, 1998)

8. J. Ohser, B. Steinbach, C. Lang

Efficient Texture Analysis of Binary Images

A new method of determining some characteristics of binary images is proposed based on a special linear filtering. This technique enables the estimation of the area fraction, the specific line length, and the specific integral of curvature. Furthermore, the specific length of the total projection is obtained, which gives detailed information about the texture of the image. The influence of lateral and directional resolution depending on the size of the applied filter mask is discussed in detail. The technique includes a method of increasing directional resolution for texture analysis while keeping lateral resolution as high as possible.
(17 pages, 1998)

9. J. Orlik

Homogenization for viscoelasticity of the integral type with aging and shrinkage

A multiphase composite with periodic distributed inclusions with a smooth boundary is considered in this contribution. The composite component materials are supposed to be linear viscoelastic and aging (of the non-convolution integral type, for which the Laplace transform with respect to time is not effectively applicable) and are subjected to isotropic shrinkage. The free shrinkage deformation can be considered as a fictitious temperature deformation in the behavior law. The procedure presented in this paper proposes a way to determine average (effective homogenized) viscoelastic and shrinkage (temperature) composite properties and the homogenized stressfield from known properties of the components. This is done by the extension of the asymptotic homogenization technique known for pure elastic nonhomogeneous bodies to the nonhomogeneous thermoviscoelasticity of the integral nonconvolution type. Up to now, the homogenization theory has not covered viscoelasticity of the integral type. SanchezPalencia (1980), Francfort & Suquet (1987) (see [2], [9]) have considered homogenization for viscoelasticity of the differential form and only up to the first derivative order. The integralmodeled viscoelasticity is more general then the differential one and includes almost all known differential models. The homogenization procedure is based on the construction of an asymptotic solution with respect to a period of the composite structure. This reduces the original problem to some auxiliary boundary value problems of elasticity and viscoelasticity on the unit periodic cell, of the same type as the original non-homogeneous problem. The existence and uniqueness results for such problems were obtained for kernels satisfying some constrain conditions. This is done by the extension of the Volterra integral operator theory to the Volterra operators with respect to the time, whose 1 kernels are space linear operators for any fixed time variables. Some ideas of such approach were proposed in [11] and [12], where the Volterra operators with kernels depending additionally on parameter were considered. This manuscript delivers results of the same nature for the case of the spaceoperator kernels.
(20 pages, 1998)

10. J. Mohring

Helmholtz Resonators with Large Aperture

The lowest resonant frequency of a cavity resonator is usually approximated by the classical Helmholtz formula. However, if the opening is rather large and the front wall is narrow this formula is no longer valid. Here we present a correction which is of third order in the ratio of the diameters of aperture and cavity. In addition to the high accuracy it allows to estimate the damping due to radiation. The result is found by applying the method of matched asymptotic expansions. The correction contains form factors describing the shapes of opening and cavity. They are computed for a number of standard geometries. Results are compared with numerical computations.
(21 pages, 1998)

11. H. W. Hamacher, A. Schöbel

On Center Cycles in Grid Graphs

Finding "good" cycles in graphs is a problem of great interest in graph theory as well as in locational analysis. We show that the center and median problems are NP hard in general graphs. This result holds both for the variable cardinality case (i.e. all cycles of the graph are considered) and the fixed cardinality case (i.e. only cycles with a given cardinality p are feasible). Hence it is of interest to investigate special cases where the problem is solvable in polynomial time. In grid graphs, the variable cardinality case is, for instance, trivially solvable if the shape of the cycle can be chosen freely. If the shape is fixed to be a rectangle one can analyze rectangles in grid graphs with, in sequence, fixed dimension, fixed cardinality, and variable cardinality. In all cases a complete characterization of the optimal cycles and closed form expressions of the optimal objective values are given, yielding polynomial time algorithms for all cases of center rectangle problems. Finally, it is shown that center cycles can be chosen as rectangles for small cardinalities such that the center cycle problem in grid graphs is in these cases completely solved.
(15 pages, 1998)

12. H. W. Hamacher, K.-H. Küfer

Inverse radiation therapy planning - a multiple objective optimisation approach

For some decades radiation therapy has been proved successful in cancer treatment. It is the major task of clinical radiation treatment planning to realize on the one hand a high level dose of radiation in the cancer tissue in order to obtain maximum tumor control. On the other hand it is obvious that it is absolutely necessary to keep in the tissue outside the tumor, particularly in organs at risk, the unavoidable radiation as low as possible.
No doubt, these two objectives of treatment planning - high level dose in the tumor, low radiation outside the tumor - have a basically contradictory nature. Therefore, it is no surprise that inverse mathematical models with dose distribution bounds tend to be infeasible in most cases. Thus, there is need for approximations compromising between overdosing the organs at risk and underdosing the target volume.
Differing from the currently used time consuming iterative approach, which measures deviation from an ideal (non-achievable) treatment plan using recursively trial-and-error weights for the organs of interest, we go a new way trying to avoid a priori weight choices and consider the treatment planning problem as a multiple objective linear programming problem: with each organ of interest, target tissue as well as organs at risk, we associate an objective function measuring the maximal deviation from the prescribed doses.
We build up a data base of relatively few efficient solutions representing and approximating the variety of Pareto solutions of the multiple objective linear programming problem. This data base can be easily scanned by physicians looking for an adequate treatment plan with the aid of an appropriate online tool.
(14 pages, 1999)

13. C. Lang, J. Ohser, R. Hilfer

On the Analysis of Spatial Binary Images

This paper deals with the characterization of microscopically heterogeneous, but macroscopically homogeneous spatial structures. A new method is presented which is strictly based on integral-geometric formulae such as Crofton's intersection formulae and Hadwiger's recursive definition of the Euler number. The corresponding algorithms have clear advantages over other techniques. As an example of application we consider the analysis of spatial digital images produced by means of Computer Assisted Tomography.
(20 pages, 1999)

14. M. Junk

On the Construction of Discrete Equilibrium Distributions for Kinetic Schemes

A general approach to the construction of discrete equilibrium distributions is presented. Such distribution functions can be used to set up Kinetic Schemes as well as Lattice Boltzmann methods. The general principles are also applied to the construction of Chapman Enskog distributions which are used in Kinetic Schemes for compressible Navier-Stokes equations.
(24 pages, 1999)

15. M. Junk, S. V. Raghurame Rao

A new discrete velocity method for Navier-Stokes equations

The relation between the Lattice Boltzmann Method, which has recently become popular, and the Kinetic Schemes, which are routinely used in Computational Fluid Dynamics, is explored. A new discrete velocity model for the numerical solution of Navier-Stokes equations for incompressible fluid flow is presented by combining both the approaches. The new scheme can be interpreted as a pseudo-compressibility method and, for a particular choice of parameters, this interpretation carries over to the Lattice Boltzmann Method.
(20 pages, 1999)

16. H. Neunzert

Mathematics as a Key to Key Technologies

The main part of this paper will consist of examples, how mathematics really helps to solve industrial problems; these examples are taken from our Institute for Industrial Mathematics, from research in the Technomathematics group at my university, but also from ECMI groups and a company called TecMath, which originated 10 years ago from my university group and has already a very successful history.
(39 pages (4 PDF-Files), 1999)

17. J. Ohser, K. Sandau

Considerations about the Estimation of the Size Distribution in Wicksell's Corpuscle Problem

Wicksell's corpuscle problem deals with the estimation of the size distribution of a population of particles, all having the same shape, using a lower dimensional sampling probe. This problem was originary formulated for particle systems occurring in life sciences but its solution is of actual and increasing interest in materials science. From a mathematical point of view, Wicksell's problem is an inverse problem where the interesting size distribution is the unknown part of a Volterra equation. The problem is often regarded ill-posed, because the structure of the integrand implies unstable numerical solutions. The accuracy of the numerical solutions is considered here using the condition number, which allows to compare different numerical methods with different (equidistant) class sizes and which indicates, as one result, that a finite section thickness of the probe reduces the numerical problems. Furthermore, the relative error of estimation is computed which can be split into two parts. One part consists of the relative discretization error that increases for increasing class size, and the second part is related to the relative statistical error which increases with decreasing class size. For both parts, upper bounds can be given and the sum of them indicates an optimal class width depending on some specific constants.
(18 pages, 1999)

18. E. Carrizosa, H. W. Hamacher, R. Klein, S. Nickel

Solving nonconvex planar location problems by finite dominating sets

It is well-known that some of the classical location problems with polyhedral gauges can be solved in polynomial time by finding a finite dominating set, i. e. a finite set of candidates guaranteed to contain at least one optimal location.
In this paper it is first established that this result holds for a much larger class of problems than currently considered in the literature. The model for which this result can be proven includes, for instance, location problems with attraction and repulsion, and location-allocation problems.
Next, it is shown that the approximation of general gauges by polyhedral ones in the objective function of our general model can be analyzed with regard to the subsequent error in the optimal objective value. For the approximation problem two different approaches are described, the sandwich procedure and the greedy algorithm. Both of these approaches lead - for fixed epsilon - to polynomial approximation algorithms with accuracy epsilon for solving the general model considered in this paper.
Keywords: Continuous Location, Polyhedral Gauges, Finite Dominating Sets, Approximation, Sandwich Algorithm, Greedy Algorithm
(19 pages, 2000)

19. A. Becker

A Review on Image Distortion Measures

Within this paper we review image distortion measures. A distortion measure is a criterion that assigns a "quality number" to an image. We distinguish between mathematical distortion measures and those distortion measures in-cooperating a priori knowledge about the imaging devices (e. g. satellite images), image processing algorithms or the human physiology. We will consider representative examples of different kinds of distortion measures and are going to discuss them.
Keywords: Distortion measure, human visual system
(26 pages, 2000)

20. H. W. Hamacher, M. Labbé, S. Nickel, T. Sonneborn

Polyhedral Properties of the Uncapacitated Multiple Allocation Hub Location Problem

We examine the feasibility polyhedron of the uncapacitated hub location problem (UHL) with multiple allocation, which has applications in the fields of air passenger and cargo transportation, telecommunication and postal delivery services. In particular we determine the dimension and derive some classes of facets of this polyhedron. We develop some general rules about lifting facets from the uncapacitated facility location (UFL) for UHL and projecting facets from UHL to UFL. By applying these rules we get a new class of facets for UHL which dominates the inequalities in the original formulation. Thus we get a new formulation of UHL whose constraints are all facet–defining. We show its superior computational performance by benchmarking it on a well known data set.
Keywords: integer programming, hub location, facility location, valid inequalities, facets, branch and cut
(21 pages, 2000)

21. H. W. Hamacher, A. Schöbel

Design of Zone Tariff Systems in Public Transportation

Given a public transportation system represented by its stops and direct connections between stops, we consider two problems dealing with the prices for the customers: The fare problem in which subsets of stops are already aggregated to zones and "good" tariffs have to be found in the existing zone system. Closed form solutions for the fare problem are presented for three objective functions. In the zone problem the design of the zones is part of the problem. This problem is NP hard and we therefore propose three heuristics which prove to be very successful in the redesign of one of Germany's transportation systems.
(30 pages, 2001)

22. D. Hietel, M. Junk, R. Keck, D. Teleaga

The Finite-Volume-Particle Method for Conservation Laws

In the Finite-Volume-Particle Method (FVPM), the weak formulation of a hyperbolic conservation law is discretized by restricting it to a discrete set of test functions. In contrast to the usual Finite-Volume approach, the test functions are not taken as characteristic functions of the control volumes in a spatial grid, but are chosen from a partition of unity with smooth and overlapping partition functions (the particles), which can even move along pre- scribed velocity fields. The information exchange between particles is based on standard numerical flux functions. Geometrical information, similar to the surface area of the cell faces in the Finite-Volume Method and the corresponding normal directions are given as integral quantities of the partition functions. After a brief derivation of the Finite-Volume-Particle Method, this work focuses on the role of the geometric coefficients in the scheme.
(16 pages, 2001)

23. T. Bender, H. Hennes, J. Kalcsics, M. T. Melo, S. Nickel

Location Software and Interface with GIS and Supply Chain Management

The objective of this paper is to bridge the gap between location theory and practice. To meet this objective focus is given to the development of software capable of addressing the different needs of a wide group of users. There is a very active community on location theory encompassing many research fields such as operations research, computer science, mathematics, engineering, geography, economics and marketing. As a result, people working on facility location problems have a very diverse background and also different needs regarding the software to solve these problems. For those interested in non-commercial applications (e. g. students and researchers), the library of location algorithms (LoLA can be of considerable assistance. LoLA contains a collection of efficient algorithms for solving planar, network and discrete facility location problems. In this paper, a detailed description of the functionality of LoLA is presented. In the fields of geography and marketing, for instance, solving facility location problems requires using large amounts of demographic data. Hence, members of these groups (e. g. urban planners and sales managers) often work with geographical information too s. To address the specific needs of these users, LoLA was inked to a geographical information system (GIS) and the details of the combined functionality are described in the paper. Finally, there is a wide group of practitioners who need to solve large problems and require special purpose software with a good data interface. Many of such users can be found, for example, in the area of supply chain management (SCM). Logistics activities involved in strategic SCM include, among others, facility location planning. In this paper, the development of a commercial location software tool is also described. The too is embedded in the Advanced Planner and Optimizer SCM software developed by SAP AG, Walldorf, Germany. The paper ends with some conclusions and an outlook to future activities.
Keywords: facility location, software development, geographical information systems, supply chain management
(48 pages, 2001)

24. H. W. Hamacher, S. A. Tjandra

Mathematical Modelling of Evacuation Problems: A State of Art

This paper details models and algorithms which can be applied to evacuation problems. While it concentrates on building evacuation many of the results are applicable also to regional evacuation. All models consider the time as main parameter, where the travel time between components of the building is part of the input and the overall evacuation time is the output. The paper distinguishes between macroscopic and microscopic evacuation models both of which are able to capture the evacuees' movement over time.
Macroscopic models are mainly used to produce good lower bounds for the evacuation time and do not consider any individual behavior during the emergency situation. These bounds can be used to analyze existing buildings or help in the design phase of planning a building. Macroscopic approaches which are based on dynamic network flow models (minimum cost dynamic flow, maximum dynamic flow, universal maximum flow, quickest path and quickest flow) are described. A special feature of the presented approach is the fact, that travel times of evacuees are not restricted to be constant, but may be density dependent. Using multicriteria optimization priority regions and blockage due to fire or smoke may be considered. It is shown how the modelling can be done using time parameter either as discrete or continuous parameter.
Microscopic models are able to model the individual evacuee's characteristics and the interaction among evacuees which influence their movement. Due to the corresponding huge amount of data one uses simulation approaches. Some probabilistic laws for individual evacuee's movement are presented. Moreover ideas to model the evacuee's movement using cellular automata (CA) and resulting software are presented.
In this paper we will focus on macroscopic models and only summarize some of the results of the microscopic approach. While most of the results are applicable to general evacuation situations, we concentrate on building evacuation.
(44 pages, 2001)

25. J. Kuhnert, S. Tiwari

Grid free method for solving the Poisson equation

A Grid free method for solving the Poisson equation is presented. This is an iterative method. The method is based on the weighted least squares approximation in which the Poisson equation is enforced to be satisfied in every iterations. The boundary conditions can also be enforced in the iteration process. This is a local approximation procedure. The Dirichlet, Neumann and mixed boundary value problems on a unit square are presented and the analytical solutions are compared with the exact solutions. Both solutions matched perfectly.
Keywords: Poisson equation, Least squares method, Grid free method
(19 pages, 2001)

26. T. Götz, H. Rave, D. Reinel-Bitzer, K. Steiner, H. Tiemeier

Simulation of the fiber spinning process

To simulate the influence of process parameters to the melt spinning process a fiber model is used and coupled with CFD calculations of the quench air flow. In the fiber model energy, momentum and mass balance are solved for the polymer mass flow. To calculate the quench air the Lattice Boltzmann method is used. Simulations and experiments for different process parameters and hole configurations are compared and show a good agreement.
Keywords: Melt spinning, fiber model, Lattice Boltzmann, CFD
(19 pages, 2001)

27. A. Zemitis

On interaction of a liquid film with an obstacle

In this paper mathematical models for liquid films generated by impinging jets are discussed. Attention is stressed to the interaction of the liquid film with some obstacle. S. G. Taylor [Proc. R. Soc. London Ser. A 253, 313 (1959)] found that the liquid film generated by impinging jets is very sensitive to properties of the wire which was used as an obstacle. The aim of this presentation is to propose a modification of the Taylor's model, which allows to simulate the film shape in cases, when the angle between jets is different from 180°. Numerical results obtained by discussed models give two different shapes of the liquid film similar as in Taylors experiments. These two shapes depend on the regime: either droplets are produced close to the obstacle or not. The difference between two regimes becomes larger if the angle between jets decreases. Existence of such two regimes can be very essential for some applications of impinging jets, if the generated liquid film can have a contact with obstacles.
Keywords: impinging jets, liquid film, models, numerical solution, shape
(22 pages, 2001)

28. I. Ginzburg, K. Steiner

Free surface lattice-Boltzmann method to model the filling of expanding cavities by Bingham Fluids

The filling process of viscoplastic metal alloys and plastics in expanding cavities is modelled using the lattice Boltzmann method in two and three dimensions. These models combine the regularized Bingham model for viscoplastic with a free-interface algorithm. The latter is based on a modified immiscible lattice Boltzmann model in which one species is the fluid and the other one is considered as vacuum. The boundary conditions at the curved liquid-vacuum interface are met without any geometrical front reconstruction from a first-order Chapman-Enskog expansion. The numerical results obtained with these models are found in good agreement with available theoretical and numerical analysis.
Keywords: Generalized LBE, free-surface phenomena, interface boundary conditions, filling processes, Bingham viscoplastic model, regularized models
(22 pages, 2001)

29. H. Neunzert

»Denn nichts ist für den Menschen als Menschen etwas wert, was er nicht mit Leidenschaft tun kann«
Vortrag anlässlich der Verleihung des Akademiepreises des Landes Rheinland-Pfalz am 21.11.2001

Was macht einen guten Hochschullehrer aus? Auf diese Frage gibt es sicher viele verschiedene, fachbezogene Antworten, aber auch ein paar allgemeine Gesichtspunkte: es bedarf der »Leidenschaft« für die Forschung (Max Weber), aus der dann auch die Begeisterung für die Lehre erwächst. Forschung und Lehre gehören zusammen, um die Wissenschaft als lebendiges Tun vermitteln zu können. Der Vortrag gibt Beispiele dafür, wie in angewandter Mathematik Forschungsaufgaben aus praktischen Alltagsproblemstellungen erwachsen, die in die Lehre auf verschiedenen Stufen (Gymnasium bis Graduiertenkolleg) einfließen; er leitet damit auch zu einem aktuellen Forschungsgebiet, der Mehrskalenanalyse mit ihren vielfältigen Anwendungen in Bildverarbeitung, Materialentwicklung und Strömungsmechanik über, was aber nur kurz gestreift wird. Mathematik erscheint hier als eine moderne Schlüsseltechnologie, die aber auch enge Beziehungen zu den Geistes- und Sozialwissenschaften hat.
Keywords: Lehre, Forschung, angewandte Mathematik, Mehrskalenanalyse, Strömungsmechanik
(18 pages, 2001)

30. J. Kuhnert, S. Tiwari

Finite pointset method based on the projection method for simulations of the incompressible Navier-Stokes equations

A Lagrangian particle scheme is applied to the projection method for the incompressible Navier-Stokes equations. The approximation of spatial derivatives is obtained by the weighted least squares method. The pressure Poisson equation is solved by a local iterative procedure with the help of the least squares method. Numerical tests are performed for two dimensional cases. The Couette flow, Poiseuelle flow, decaying shear flow and the driven cavity flow are presented. The numerical solutions are obtained for stationary as well as instationary cases and are compared with the analytical solutions for channel flows. Finally, the driven cavity in a unit square is considered and the stationary solution obtained from this scheme is compared with that from the finite element method.
Keywords: Incompressible Navier-Stokes equations, Meshfree method, Projection method, Particle scheme, Least squares approximation
AMS subject classification: 76D05, 76M28
(25 pages, 2001)

31. R. Korn, M. Krekel

Optimal Portfolios with Fixed Consumption or Income Streams

We consider some portfolio optimisation problems where either the investor has a desire for an a priori specified consumption stream or/and follows a deterministic pay in scheme while also trying to maximize expected utility from final wealth. We derive explicit closed form solutions for continuous and discrete monetary streams. The mathematical method used is classical stochastic control theory.
Keywords: Portfolio optimisation, stochastic control, HJB equation, discretisation of control problems.
(23 pages, 2002)

32. M. Krekel

Optimal portfolios with a loan dependent credit spread

If an investor borrows money he generally has to pay higher interest rates than he would have received, if he had put his funds on a savings account. The classical model of continuous time portfolio optimisation ignores this effect. Since there is obviously a connection between the default probability and the total

percentage of wealth, which the investor is in debt, we study portfolio optimisation with a control dependent interest rate. Assuming a logarithmic and a power utility function, respectively, we prove explicit formulae of the optimal control.
Keywords: Portfolio optimisation, stochastic control, HJB equation, credit spread, log utility, power utility, non-linear wealth dynamics
(25 pages, 2002)

33. J. Ohser, W. Nagel, K. Schladitz

The Euler number of discretized sets - on the choice of adjacency in homogeneous lattices

Two approaches for determining the Euler-Poincaré characteristic of a set observed on lattice points are considered in the context of image analysis { the integral geometric and the polyhedral approach. Information about the set is assumed to be available on lattice points only. In order to retain properties of the Euler number and to provide a good approximation of the true Euler number of the original set in the Euclidean space, the appropriate choice of adjacency in the lattice for the set and its background is crucial. Adjacencies are defined using tessellations of the whole space into polyhedrons. In R 3 , two new 14 adjacencies are introduced additionally to the well known 6 and 26 adjacencies. For the Euler number of a set and its complement, a consistency relation holds. Each of the pairs of adjacencies (14:1; 14:1), (14:2; 14:2), (6; 26), and (26; 6) is shown to be a pair of complementary adjacencies with respect to this relation. That is, the approximations of the Euler numbers are consistent if the set and its background (complement) are equipped with this pair of adjacencies. Furthermore, sufficient conditions for the correctness of the approximations of the Euler number are given. The analysis of selected microstructures and a simulation study illustrate how the estimated Euler number depends on the chosen adjacency. It also shows that there is not a uniquely best pair of adjacencies with respect to the estimation of the Euler number of a set in Euclidean space.
Keywords: image analysis, Euler number, neighborhod relationships, cuboidal lattice
(32 pages, 2002)

34. I. Ginzburg, K. Steiner

Lattice Boltzmann Model for Free-Surface flow and Its Application to Filling Process in Casting

A generalized lattice Boltzmann model to simulate free-surface is constructed in both two and three dimensions. The proposed model satisfies the interfacial boundary conditions accurately. A distinctive feature of the model is that the collision processes is carried out only on the points occupied partially or fully by the fluid. To maintain a sharp interfacial front, the method includes an anti-diffusion algorithm. The unknown distribution functions at the interfacial region are constructed according to the first order Chapman-Enskog analysis. The interfacial boundary conditions are satisfied exactly by the coefficients in the Chapman-Enskog expansion. The distribution functions are naturally expressed in the local interfacial coordinates. The macroscopic quantities at the interface are extracted from the least-square solutions of a locally linearized system obtained from the known distribution functions. The proposed method does not require any geometric front construction and is robust for any interfacial topology. Simulation results of realistic filling process are presented: rectangular cavity in two dimensions and Hammer box, Campbell box, Sheffield box, and Motorblock in three dimensions. To enhance the stability at high Reynolds numbers, various upwind-type schemes are developed. Free-slip and no-slip boundary conditions are also discussed.
Keywords: Lattice Boltzmann models; free-surface phenomena; interface boundary conditions; filling processes; injection molding; volume of fluid method; interface boundary conditions; advection-schemes; upwind-schemes
(54 pages, 2002)

35. M. Günther, A. Klar, T. Materne, R. Wegener

Multivalued fundamental diagrams and stop and go waves for continuum traffic equations

In the present paper a kinetic model for vehicular traffic leading to multivalued fundamental diagrams is developed and investigated in detail. For this model phase transitions can appear depending on the local density and velocity of the flow. A derivation of associated macroscopic traffic equations from the kinetic equation is given. Moreover, numerical experiments show the appearance of stop and go waves for highway traffic with a bottleneck.
Keywords: traffic flow, macroscopic equations, kinetic derivation, multivalued fundamental diagram, stop and go waves, phase transitions
(25 pages, 2002)

36. S. Feldmann, P. Lang, D. Prätzel-Wolters

Parameter influence on the zeros of network determinants

To a network N(q) with determinant D(s;q) depending on a parameter vector q Î Rr via identification of some of its vertices, a network N^ (q) is assigned. The paper deals with procedures to find N^ (q), such that its determinant D^ (s;q) admits a factorization in the determinants of appropriate subnetworks, and with the estimation of the deviation of the zeros of D^ from the zeros of D. To solve the estimation problem state space methods are applied.
Keywords: Networks, Equicofactor matrix polynomials, Realization theory, Matrix perturbation theory
(30 pages, 2002)

37. K. Koch, J. Ohser, K. Schladitz

Spectral theory for random closed sets and estimating the covariance via frequency space

A spectral theory for stationary random closed sets is developed and provided with a sound mathematical basis. Definition and proof of existence of the Bartlett spectrum of a stationary random closed set as well as the proof of a Wiener-Khintchine theorem for the power spectrum are used to two ends: First, well known second order characteristics like the covariance can be estimated faster than usual via frequency space. Second, the Bartlett spectrum and the power spectrum can be used as second order characteristics in frequency space. Examples show, that in some cases information about the random closed set is easier to obtain from these characteristics in frequency space than from their real world counterparts.
Keywords: Random set, Bartlett spectrum, fast Fourier transform, power spectrum
(28 pages, 2002)

38. D. d'Humières, I. Ginzburg

Multi-reflection boundary conditions for lattice Boltzmann models

We present a unified approach of several boundary conditions for lattice Boltzmann models. Its general framework is a generalization of previously introduced schemes such as the bounce-back rule, linear or quadratic interpolations, etc. The objectives are two fold: first to give theoretical tools to study the existing boundary conditions and their corresponding accuracy; secondly to design formally third- order accurate boundary conditions for general flows. Using these boundary conditions, Couette and Poiseuille flows are exact solution of the lattice Boltzmann models for a Reynolds number Re = 0 (Stokes limit).
Numerical comparisons are given for Stokes flows in periodic arrays of spheres and cylinders, linear periodic array of cylinders between moving plates and for Navier-Stokes flows in periodic arrays of cylinders for Re < 200. These results show a significant improvement of the overall accuracy when using the linear interpolations instead of the bounce-back reflection (up to an order of magnitude on the hydrodynamics fields). Further improvement is achieved with the new multi-reflection boundary conditions, reaching a level of accuracy close to the quasi-analytical reference solutions, even for rather modest grid resolutions and few points in the narrowest channels. More important, the pressure and velocity fields in the vicinity of the obstacles are much smoother with multi-reflection than with the other boundary conditions.
Finally the good stability of these schemes is highlighted by some simulations of moving obstacles: a cylinder between flat walls and a sphere in a cylinder.
Keywords: lattice Boltzmann equation, boudary condistions, bounce-back rule, Navier-Stokes equation
(72 pages, 2002)

39. R. Korn

Elementare Finanzmathematik

Im Rahmen dieser Arbeit soll eine elementar gehaltene Einführung in die Aufgabenstellungen und Prinzipien der modernen Finanzmathematik gegeben werden. Insbesondere werden die Grundlagen der Modellierung von Aktienkursen, der Bewertung von Optionen und der Portfolio-Optimierung vorgestellt. Natürlich können die verwendeten Methoden und die entwickelte Theorie nicht in voller Allgemeinheit für den Schulunterricht verwendet werden, doch sollen einzelne Prinzipien so heraus gearbeitet werden, dass sie auch an einfachen Beispielen verstanden werden können.
Keywords: Finanzmathematik, Aktien, Optionen, Portfolio-Optimierung, Börse, Lehrerweiterbildung, Mathematikunterricht
(98 pages, 2002)

40. J. Kallrath, M. C. Müller, S. Nickel

Batch Presorting Problems: Models and Complexity Results

In this paper we consider short term storage systems. We analyze presorting strategies to improve the effiency of these storage systems. The presorting task is called Batch PreSorting Problem (BPSP). The BPSP is a variation of an assigment problem, i.e., it has an assigment problem kernel and some additional constraints. We present different types of these presorting problems, introduce mathematical programming formulations and prove the NP-completeness for one type of the BPSP. Experiments are carried out in order to compare the different model formulations and to investigate the behavior of these models.
Keywords: Complexity theory, Integer programming, Assigment, Logistics
(19 pages, 2002)

41. J. Linn

On the frame-invariant description of the phase space of the Folgar-Tucker equation

The Folgar-Tucker equation is used in flow simulations of fiber suspensions to predict fiber orientation depending on the local flow. In this paper, a complete, frame-invariant description of the phase space of this differential equation is presented for the first time.
Key words: fiber orientation, Folgar-Tucker equation, injection molding
(5 pages, 2003)

42. T. Hanne, S. Nickel

A Multi-Objective Evolutionary Algorithm for Scheduling and Inspection Planning in Software Development Projects

In this article, we consider the problem of planning inspections and other tasks within a software development (SD) project with respect to the objectives quality (no. of defects), project duration, and costs. Based on a discrete-event simulation model of SD processes comprising the phases coding, inspection, test, and rework, we present a simplified formulation of the problem as a multiobjective optimization problem. For solving the problem (i.e. finding an approximation of the efficient set) we develop a multiobjective evolutionary algorithm. Details of the algorithm are discussed as well as results of its application to sample problems.
Key words: multiple objective programming, project management and scheduling, software development, evolutionary algorithms, efficient set
(29 pages, 2003)

43. T. Bortfeld , K.-H. Küfer, M. Monz, A. Scherrer, C. Thieke, H. Trinkaus

Intensity-Modulated Radiotherapy - A Large Scale Multi-Criteria Programming Problem -

Radiation therapy planning is always a tight rope walk between dangerous insufficient dose in the target volume and life threatening overdosing of organs at risk. Finding ideal balances between these inherently contradictory goals challenges dosimetrists and physicians in their daily practice. Today's planning systems are typically based on a single evaluation function that measures the quality of a radiation treatment plan. Unfortunately, such a one dimensional approach cannot satisfactorily map the different backgrounds of physicians and the patient dependent necessities. So, too often a time consuming iteration process between evaluation of dose distribution and redefinition of the evaluation function is needed.
In this paper we propose a generic multi-criteria approach based on Pareto's solution concept. For each entity of interest - target volume or organ at risk a structure dependent evaluation function is defined measuring deviations from ideal doses that are calculated from statistical functions. A reasonable bunch of clinically meaningful Pareto optimal solutions are stored in a data base, which can be interactively searched by physicians. The system guarantees dynamical planning as well as the discussion of tradeoffs between different entities.
Mathematically, we model the upcoming inverse problem as a multi-criteria linear programming problem. Because of the large scale nature of the problem it is not possible to solve the problem in a 3D-setting without adaptive reduction by appropriate approximation schemes.
Our approach is twofold: First, the discretization of the continuous problem is based on an adaptive hierarchical clustering process which is used for a local refinement of constraints during the optimization procedure. Second, the set of Pareto optimal solutions is approximated by an adaptive grid of representatives that are found by a hybrid process of calculating extreme compromises and interpolation methods.
Keywords: multiple criteria optimization, representative systems of Pareto solutions, adaptive triangulation, clustering and disaggregation techniques, visualization of Pareto solutions, medical physics, external beam radiotherapy planning, intensity modulated radiotherapy
(31 pages, 2003)

44. T. Halfmann, T. Wichmann

Overview of Symbolic Methods in Industrial Analog Circuit Design

Industrial analog circuits are usually designed using numerical simulation tools. To obtain a deeper circuit understanding, symbolic analysis techniques can additionally be applied. Approximation methods which reduce the complexity of symbolic expressions are needed in order to handle industrial-sized problems. This paper will give an overview to the field of symbolic analog circuit analysis. Starting with a motivation, the state-of-the-art simplification algorithms for linear as well as for nonlinear circuits are presented. The basic ideas behind the different techniques are described, whereas the technical details can be found in the cited references. Finally, the application of linear and nonlinear symbolic analysis will be shown on two example circuits.
Keywords: CAD, automated analog circuit design, symbolic analysis, computer algebra, behavioral modeling, system simulation, circuit sizing, macro modeling, differential-algebraic equations, index
(17 pages, 2003)

45. S. E. Mikhailov, J. Orlik

Asymptotic Homogenisation in Strength and Fatigue Durability Analysis of Composites

Asymptotic homogenisation technique and two-scale convergence is used for analysis of macro-strength and fatigue durability of composites with a periodic structure under cyclic loading. The linear damage accumulation rule is employed in the phenomenological micro-durability conditions (for each component of the composite) under varying cyclic loading. Both local and non-local strength and durability conditions are analysed. The strong convergence of the strength and fatigue damage measure as the structure period tends to zero is proved and their limiting values are estimated.
Keywords: multiscale structures, asymptotic homogenization, strength, fatigue, singularity, non-local conditions
(14 pages, 2003)

46. P. Domínguez-Marín, P. Hansen, N. Mladenovi´c , S. Nickel

Heuristic Procedures for Solving the Discrete Ordered Median Problem

We present two heuristic methods for solving the Discrete Ordered Median Problem (DOMP), for which no such approaches have been developed so far. The DOMP generalizes classical discrete facility location problems, such as the p-median, p-center and Uncapacitated Facility Location problems. The first procedure proposed in this paper is based on a genetic algorithm developed by Moreno Vega [MV96] for p-median and p-center problems. Additionally, a second heuristic approach based on the Variable Neighborhood Search metaheuristic (VNS) proposed by Hansen & Mladenovic [HM97] for the p-median problem is described. An extensive numerical study is presented to show the efficiency of both heuristics and compare them.
Keywords: genetic algorithms, variable neighborhood search, discrete facility location
(31 pages, 2003)

47. N. Boland, P. Domínguez-Marín, S. Nickel, J. Puerto

Exact Procedures for Solving the Discrete Ordered Median Problem

The Discrete Ordered Median Problem (DOMP) generalizes classical discrete location problems, such as the N-median, N-center and Uncapacitated Facility Location problems. It was introduced by Nickel [16], who formulated it as both a nonlinear and a linear integer program. We propose an alternative integer linear programming formulation for the DOMP, discuss relationships between both integer linear programming formulations, and show how properties of optimal solutions can be used to strengthen these formulations. Moreover, we present a specific branch and bound procedure to solve the DOMP more efficiently. We test the integer linear programming formulations and this branch and bound method computationally on randomly generated test problems.
Keywords: discrete location, Integer programming
(41 pages, 2003)

48. S. Feldmann, P. Lang

Padé-like reduction of stable discrete linear systems preserving their stability

A new stability preserving model reduction algorithm for discrete linear SISO-systems based on their impulse response is proposed. Similar to the Padé approximation, an equation system for the Markov parameters involving the Hankel matrix is considered, that here however is chosen to be of very high dimension. Although this equation system therefore in general cannot be solved exactly, it is proved that the approximate solution, computed via the Moore-Penrose inverse, gives rise to a stability preserving reduction scheme, a property that cannot be guaranteed for the Padé approach. Furthermore, the proposed algorithm is compared to another stability preserving reduction approach, namely the balanced truncation method, showing comparable performance of the reduced systems. The balanced truncation method however starts from a state space description of the systems and in general is expected to be more computational demanding.
Keywords: Discrete linear systems, model reduction, stability, Hankel matrix, Stein equation
(16 pages, 2003)

49. J. Kallrath, S. Nickel

A Polynomial Case of the Batch Presorting Problem

This paper presents new theoretical results for a special case of the batch presorting problem (BPSP). We will show tht this case can be solved in polynomial time. Offline and online algorithms are presented for solving the BPSP. Competetive analysis is used for comparing the algorithms.
Keywords: batch presorting problem, online optimization, competetive analysis, polynomial algorithms, logistics
(17 pages, 2003)

50. T. Hanne, H. L. Trinkaus

***knowCube for MCDM –
Visual and Interactive Support for Multicriteria Decision Making***

In this paper, we present a novel multicriteria decision support system (MCDSS), called knowCube, consisting of components for knowledge organization, generation, and navigation. Knowledge organization rests upon a database for managing qualitative and quantitative criteria, together with add-on information. Knowledge generation serves filling the database via e. g. identification, optimization, classification or simulation. For "finding needles in haycocks", the knowledge navigation component supports graphical database retrieval and interactive, goal-oriented problem solving. Navigation "helpers" are, for instance, cascading criteria aggregations, modifiable metrics, ergonomic interfaces, and customizable visualizations. Examples from real-life projects, e.g. in industrial engineering and in the life sciences, illustrate the application of our MCDSS.
Key words: Multicriteria decision making, knowledge management, decision support systems, visual interfaces, interactive navigation, real-life applications.
(26 pages, 2003)

51. O. Iliev, V. Laptev

On Numerical Simulation of Flow Through Oil Filters

This paper concerns numerical simulation of flow through oil filters. Oil filters consist of filter housing (filter box), and a porous filtering medium, which completely separates the inlet from the outlet. We discuss mathematical models, describing coupled flows in the pure liquid subregions and in the porous filter media, as well as interface conditions between them. Further, we reformulate the problem in fictitious regions method manner, and discuss peculiarities of the numerical algorithm in solving the coupled system. Next, we show numerical results, validating the model and the algorithm. Finally, we present results from simulation of 3-D oil flow through a real car filter.
Keywords: oil filters, coupled flow in plain and porous media, Navier-Stokes, Brinkman, numerical simulation
(8 pages, 2003)

52. W. Dörfler, O. Iliev, D. Stoyanov, D. Vassileva

On a Multigrid Adaptive Refinement Solver for Saturated Non-Newtonian Flow in Porous Media

A multigrid adaptive refinement algorithm for non-Newtonian flow in porous media is presented. The saturated flow of a non-Newtonian fluid is described by the continuity equation and the generalized Darcy law. The resulting second order nonlinear elliptic equation is discretized by a finite volume method on a cell-centered grid. A nonlinear full-multigrid, full-approximation-storage algorithm is implemented. As a smoother, a single grid solver based on Picard linearization and Gauss-Seidel relaxation is used. Further, a local refinement multigrid algorithm on a composite grid is developed. A residual based error indicator is used in the adaptive refinement criterion. A special implementation approach is used, which allows us to perform unstructured local refinement in conjunction with the finite volume discretization. Several results from numerical experiments are presented in order to examine the performance of the solver.
Keywords: Nonlinear multigrid, adaptive refinement, non-Newtonian flow in porous media
(17 pages, 2003)

53. S. Kruse

On the Pricing of Forward Starting Options under Stochastic Volatility

We consider the problem of pricing European forward starting options in the presence of stochastic volatility. By performing a change of measure using the asset price at the time of strike determination as a numeraire, we derive a closed-form solution based on Heston's model of stochastic volatility.

Keywords: Option pricing, forward starting options, Heston model, stochastic volatility, cliquet options

(11 pages, 2003)

54. O. Iliev, D. Stoyanov

Multigrid – adaptive local refinement solver for incompressible flows

A non-linear multigrid solver for incompressible Navier-Stokes equations, exploiting finite volume discretization of the equations, is extended by adaptive local refinement. The multigrid is the outer iterative cycle, while the SIMPLE algorithm is used as a smoothing procedure. Error indicators are used to define the refinement subdomain. A special implementation approach is used, which allows to perform unstructured local refinement in conjunction with the finite volume discretization. The multigrid - adaptive local refinement algorithm is tested on 2D Poisson equation and further is applied to a lid-driven flows in a cavity (2D and 3D case), comparing the results with bench-mark data. The software design principles of the solver are also discussed.

Keywords: Navier-Stokes equations, incompressible flow, projection-type splitting, SIMPLE, multigrid methods, adaptive local refinement, lid-driven flow in a cavity

(37 pages, 2003)

55. V. Starikovicius

The multiphase flow and heat transfer in porous media

In first part of this work, summaries of traditional Multiphase Flow Model and more recent Multiphase Mixture Model are presented. Attention is being paid to attempts include various heterogeneous aspects into models. In second part, MMM based differential model for two-phase immiscible flow in porous media is considered. A numerical scheme based on the sequential solution procedure and control volume based finite difference schemes for the pressure and saturation-conservation equations is developed. A computer simulator is built, which exploits object-oriented programming techniques. Numerical result for several test problems are reported.

Keywords: Two-phase flow in porous media, various formulations, global pressure, multiphase mixture model, numerical simulation

(30 pages, 2003)

56. P. Lang, A. Sarishvili, A. Wirsen

Blocked neural networks for knowledge extraction in the software development process

One of the main goals of an organization developing software is to increase the quality of the software while at the same time to decrease the costs and the duration of the development process. To achieve this, various decisions e.ecting this goal before and during the development process have to be made by the managers. One appropriate tool for decision support are simulation models of the software life cycle, which also help to understand the dynamics of the software development process. Building up a simulation model requires a mathematical description of the interactions between di.erent objects involved in the development process. Based on experimental data, techniques from the .eld of knowledge discovery can be used to quantify these interactions and to generate new process knowledge based on the analysis of the determined relationships. In this paper blocked neuronal networks and related relevance measures will be presented as an appropriate tool for quanti.cation and validation of qualitatively known dependencies in the software development process.

Keywords: Blocked Neural Networks, Nonlinear Regression, Knowledge Extraction, Code Inspection

(21 pages, 2003)

57. H. Knaf, P. Lang, S. Zeiser

Diagnosis aiding in Regulation Thermography using Fuzzy Logic

The objective of the present article is to give an overview of an application of Fuzzy Logic in Regulation Thermography, a method of medical diagnosis support. An introduction to this method of the complementary medical science based on temperature measurements – so-called thermograms – is provided. The process of modelling the physician's thermogram evaluation rules using the calculus of Fuzzy Logic is explained.

Keywords: fuzzy logic,knowledge representation, expert system

(22 pages, 2003)

58. M.T. Melo, S. Nickel, F. Saldanha da Gama

Largescale models for dynamic multi-commodity capacitated facility location

In this paper we focus on the strategic design of supply chain networks. We propose a mathematical modeling framework that captures many practical aspects of network design problems simultaneously but which have not received adequate attention in the literature. The aspects considered include: dynamic planning horizon, generic supply chain network structure, external supply of materials, inventory opportunities for goods, distribution of commodities, facility configuration, availability of capital for investments, and storage limitations. Moreover, network configuration decisions concerning the gradual relocation of facilities over the planning horizon are considered. To cope with fluctuating demands, capacity expansion and reduction scenarios are also analyzed as well as modular capacity shifts. The relation of the proposed modeling framework with existing models is discussed. For problems of reasonable size we report on our computational experience with standard mathematical programming software. In particular, useful insights on the impact of various factors on network design decisions are provided.

Keywords: supply chain management, strategic planning, dynamic location, modeling

(40 pages, 2003)

59. J. Orlik

Homogenization for contact problems with periodically rough surfaces

We consider the contact of two elastic bodies with rough surfaces at the interface. The size of the micropeaks and valleys is very small compared with the macrosize of the bodies' domains. This makes the direct application of the FEM for the calculation of the contact problem prohibitively costly. A method is developed that allows deriving a macrocontact condition on the interface. The method involves the twoscale asymptotic homogenization procedure that takes into account the microgeometry of the interface layer and the stiffnesses of materials of both domains. The macrocontact condition can then be used in a FEM model for the contact problem on the macrolevel. The averaged contact stiffness obtained allows the replacement of the interface layer in the macromodel by the macrocontact condition.

Keywords: asymptotic homogenization, contact problems

(28 pages, 2004)

60. A. Scherrer, K.-H. Küfer, M. Monz, F. Alonso, T. Bortfeld

IMRT planning on adaptive volume structures – a significant advance of computational complexity

In intensity-modulated radiotherapy (IMRT) planning the oncologist faces the challenging task of finding a treatment plan that he considers to be an ideal compromise of the inherently contradictive goals of delivering a sufficiently high dose to the target while widely sparing critical structures. The search for this a priori unknown compromise typically requires the computation of several plans, i.e. the solution of several optimization problems. This accumulates to a high computational expense due to the large scale of these problems - a consequence of the discrete problem formulation. This paper presents the adaptive clustering method as a new algorithmic concept to overcome these difficulties. The computations are performed on an individually adapted structure of voxel clusters rather than on the original voxels leading to a decisively reduced computational complexity as numerical examples on real clinical data demonstrate. In contrast to many other similar concepts, the typical trade-off between a reduction in computational complexity and a loss in exactness can be avoided: the adaptive clustering method produces the optimum of the original problem. This flexible method can be applied to both single- and multi-criteria optimization methods based on most of the convex evaluation functions used in practice.

Keywords: Intensity-modulated radiation therapy (IMRT), inverse treatment planning, adaptive volume structures, hierarchical clustering, local refinement, adaptive clustering, convex programming, mesh generation, multi-grid methods

(24 pages, 2004)

61. D. Kehrwald

Parallel lattice Boltzmann simulation of complex flows

After a short introduction to the basic ideas of lattice Boltzmann methods and a brief description of a modern parallel computer, it is shown how lattice Boltzmann schemes are successfully applied for simulating fluid flow in microstructures and calculating material properties of porous media. It is explained how lattice Boltzmann schemes compute the gradient of the velocity field without numerical differentiation. This feature is then utilised for the simulation of pseudo-plastic fluids, and numerical results are presented for a simple benchmark problem as well as for the simulation of liquid composite moulding.

Keywords: Lattice Boltzmann methods, parallel computing, microstructure simulation, virtual material design, pseudo-plastic fluids, liquid composite moulding

(12 pages, 2004)

62. O. Iliev, J. Linn, M. Moog, D. Niedziela, V. Starikovicius

On the Performance of Certain Iterative Solvers for Coupled Systems Arising in Discretization of Non-Newtonian Flow Equations

Iterative solution of large scale systems arising after discretization and linearization of the unsteady non-Newtonian Navier–Stokes equations is studied. cross WLF model is used to account for the non-Newtonian behavior of the fluid. Finite volume method is used to discretize the governing system of PDEs. Viscosity is treated explicitely (e.g., it is taken from the previous time step), while other terms are treated implicitly. Different preconditioners (block–diagonal, block–triangular, relaxed incomplete LU factorization, etc.) are used in conjunction with advanced iterative methods, namely, BiCGStab, CGS, GMRES. The action of the preconditioner in fact requires inverting different blocks. For this purpose, in addition to preconditioned BiCGStab, CGS, GMRES, we use also algebraic multigrid method (AMG). The performance of the iterative solvers is studied with respect to the number of unknowns, characteristic velocity in the basic flow, time step, deviation from Newtonian behavior, etc. Results from numerical experiments are presented and discussed.

Keywords: Performance of iterative solvers, Preconditioners, Non-Newtonian flow

(17 pages, 2004)

63. R. Ciegis, O. Iliev, S. Rief, K. Steiner

On Modelling and Simulation of Different Regimes for Liquid Polymer Moulding

In this paper we consider numerical algorithms for solving a system of nonlinear PDEs arising in modeling of liquid polymer injection. We investigate the particular case when a porous preform is located within the mould, so that the liquid polymer flows through a porous medium during the filling stage. The nonlinearity of the governing system of PDEs is due to the non-Newtonian behavior of the polymer, as well as due to the moving free boundary. The latter is related to the penetration front and a Stefan type problem is formulated to account for it. A finite-volume method is used

to approximate the given differential problem. Results of numerical experiments are presented.
We also solve an inverse problem and present algorithms for the determination of the absolute preform permeability coefficient in the case when the velocity of the penetration front is known from measurements. In both cases (direct and inverse problems) we emphasize on the specifics related to the non-Newtonian behavior of the polymer. For completeness, we discuss also the Newtonian case. Results of some experimental measurements are presented and discussed.
Keywords: Liquid Polymer Moulding, Modelling, Simulation, Infiltration, Front Propagation, non-Newtonian flow in porous media
(43 pages, 2004)

64. T. Hanne, H. Neu

Simulating Human Resources in Software Development Processes

In this paper, we discuss approaches related to the explicit modeling of human beings in software development processes. While in most older simulation models of software development processes, esp. those of the system dynamics type, humans are only represented as a labor pool, more recent models of the discrete-event simulation type require representations of individual humans. In that case, particularities regarding the person become more relevant. These individual effects are either considered as stochastic variations of productivity, or an explanation is sought based on individual characteristics, such as skills for instance. In this paper, we explore such possibilities by recurring to some basic results in psychology, sociology, and labor science. Various specific models for representing human effects in software process simulation are discussed.
Keywords: Human resource modeling, software process, productivity, human factors, learning curve
(14 pages, 2004)

65. O. Iliev, A. Mikelic, P. Popov

Fluid structure interaction problems in deformable porous media: Toward permeability of deformable porous media

In this work the problem of fluid flow in deformable porous media is studied. First, the stationary fluid-structure interaction (FSI) problem is formulated in terms of incompressible Newtonian fluid and a linearized elastic solid. The flow is assumed to be characterized by very low Reynolds number and is described by the Stokes equations. The strains in the solid are small allowing for the solid to be described by the Lame equations, but no restrictions are applied on the magnitude of the displacements leading to strongly coupled, nonlinear fluid-structure problem. The FSI problem is then solved numerically by an iterative procedure which solves sequentially fluid and solid subproblems. Each of the two subproblems is discretized by finite elements and the fluid-structure coupling is reduced to an interface boundary condition. Several numerical examples are presented and the results from the numerical computations are used to perform permeability computations for different geometries.
Keywords: fluid-structure interaction, deformable porous media, upscaling, linear elasticity, stokes, finite elements
(23 pages, 2004)

66. F. Gaspar, O. Iliev, F. Lisbona, A. Naumovich, P. Vabishchevich

On numerical solution of 1-D poroelasticity equations in a multilayered domain

Finite volume discretization of Biot system of poroelasticity in a multilayered domain is presented. Staggered grid is used in order to avoid nonphysical oscillations of the numerical solution, appearing when a collocated grid is used. Various numerical experiments are presented in order to illustrate the accuracy of the finite difference scheme. In the first group of experiments, problems having analytical solutions are solved, and the order of convergence for the velocity, the pressure, the displacements, and the stresses is analyzed. In the second group of experiments numerical solution of real problems is presented.
Keywords: poroelasticity, multilayered material, finite volume discretization, MAC type grid
(41 pages, 2004)

67. J. Ohser, K. Schladitz, K. Koch, M. Nöthe

Diffraction by image processing and its application in materials science

A spectral theory for constituents of macroscopically homogeneous random microstructures modeled as homogeneous random closed sets is developed and provided with a sound mathematical basis, where the spectrum obtained by Fourier methods corresponds to the angular intensity distribution of x-rays scattered by this constituent. It is shown that the fast Fourier transform applied to three-dimensional images of microstructures obtained by micro-tomography is a powerful tool of image processing. The applicability of this technique is is demonstrated in the analysis of images of porous media.
Keywords: porous microstructure, image analysis, random set, fast Fourier transform, power spectrum, Bartlett spectrum
(13 pages, 2004)

68. H. Neunzert

Mathematics as a Technology: Challenges for the next 10 Years

No doubt: Mathematics has become a technology in its own right, maybe even a key technology. Technology may be defined as the application of science to the problems of commerce and industry. And science? Science maybe defined as developing, testing and improving models for the prediction of system behavior; the language used to describe these models is mathematics and mathematics provides methods to evaluate these models. Here we are! Why has mathematics become a technology only recently? Since it got a tool, a tool to evaluate complex, “near to reality” models: Computer! The model may be quite old – Navier-Stokes equations describe flow behavior rather well, but to solve these equations for realistic geometry and higher Reynolds numbers with sufficient precision is even for powerful parallel computing a real challenge. Make the models as simple as possible, as complex as necessary – and then evaluate them with the help of efficient and reliable algorithms: These are genuine mathematical tasks.
Keywords: applied mathematics, technology, modelling, simulation, visualization, optimization, glass processing, spinning processes, fiber-fluid interaction, trubulence effects, topological optimization, multicriteria optimization, Uncertainty and Risk, financial mathematics, Malliavin calculus, Monte-Carlo methods, virtual material design, filtration, bio-informatics, system biology
(29 pages, 2004)

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