



**Fraunhofer** Institut  
Techno- und  
Wirtschaftsmathematik

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Diagnosis aiding in Regulation  
Thermography using Fuzzy Logic

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ISSN 1434-9973

Bericht 57 (2003)

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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



# Diagnosis aiding in Regulation Thermography using Fuzzy Logic

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August 2003

## Abstract

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.

## 1 Introduction

Fuzzy Logic is an extension of Boolean Logic: logical statements in Boolean Logic are either true or false. In Fuzzy Logic every such statement has a truth value typically lying in the interval  $[0, 1] \subset \mathbb{R}$ , where the value 0 represents a false while 1 is assigned to a true statement. Truth values like 0.5 or 0.8 reflect the degree of belief in certain statements occurring for example in the medical science or in Quantum Physics.

Clearly when passing from binary to multi-valued logic the logical operators  $\vee$  (OR),  $\wedge$  (AND) and  $\neg$  (NEGATION) must be redefined. The same is true for the logical implication  $A \Rightarrow B$ , where  $A, B$  are two logical statements. It turns out that there are infinitely many ways to extend the boolean logical operators. The concrete choice depends on the specific situation in which Fuzzy Logic is applied.

Throughout the present article we will assume some familiarity of the reader with the basic concepts of Fuzzy Logic as found in introductory books like [1] or [4]. More specialized expositions are [3] or [5].

Fuzzy Logic can be applied in various ways and in a variety of areas. In the context of diagnosis support that we describe in the present article, Fuzzy Logic provides a convenient way for the representation of human knowledge within an Expert System.

An Expert System can be defined as a collection of data and rules to deal with this data, that allows to simulate an expert in a specific field. Such a system could for example consist of the precise description of a method for the diagnosis of malaria. In this sense every book on the diagnosis of tropical diseases is an Expert System. However usually this term is used in the more restricted sense of a software package into which data and rules are implemented, and that allows

the user to »simulate the expert« by running the program as well as to view and edit data and rules.

We should mention at this point that the approach to Expert Systems just described is called »rule-based« in contrast to the »object oriented« one. We will utilize the rule-based approach throughout the whole article.

When building an Expert System the problem of formally representing the expert's knowledge in a convenient way within the system arises. Here the adjective »convenient« means that the formal representation should be easy to read and to understand for the experts in the considered field, as to allow them direct access to the knowledge stored in the system. Depending on the type of knowledge Fuzzy Logic provides a possible solution for this representation problem.

Usually the calculus of Fuzzy Logic is not only used to represent expert knowledge within a system, but the representation is coupled with software that allows to compute the truth values of statements formulated in this calculus – a so-called Fuzzy Inference System.

Medical diagnosis is a typical field of application for various types of Expert Systems: on one hand the daily work of a physician produces a large amount of data that can be used to test existing or to establish new medical hypothesis. On the other hand long-term experience often yields extensive systems of rules helping in the task of early and secure detection of specific diseases. In this situation an Expert System can be useful in several ways. It serves as an easy to use database that allows to run simulations based on the incorporated knowledge. Novices may use it in their training. Groups of scientists can share one Expert System thus facilitating the process of objectifying knowledge. These examples do only form a part of the possible applications.

Regulation Thermography is a diagnostic method that utilizes the behavior of the human body's skin temperature distribution under the influence of a cold stimulus. The observed temperature patterns are classified according to their types and degrees of pathology. Eventually a set of interpretation rules is applied to gain diagnostic statements. The whole process is based on a double measurement of the skin temperature at 110 locations (»areas«) of the body leading to a so-called thermogram. The temperature at each area is measured before and a certain time after the cold stimulus. The interpretation rules involve both the absolute temperature values and the differences between the measurements before and after the cold stimulus.

At present Regulation Thermography as a method is not generally accepted among physicians partly due to the fact that its diagnostic power is not yet verified by standard medical means. However especially in the field of female breast cancer diagnosis some effort is going on to improve this situation. One activity in this trial consists of the BMBF-project »Datenbasierte Diagnoseunterstützung in der Regulationsthermographie« having the aim to implement a complete set of thermogram interpretation rules for the diagnosis of female breast cancer into a rule-based Expert System using Fuzzy Logic and Neural Nets.

At the time of writing this article approximately 130 interpretation rules as used by thermographers have been incorporated into a Fuzzy Inference System. This system takes the 220 values of a thermogram as input and determines a »probability« for the presence of a Mamma Carcinome on a 6-stage scale. In

the sequel this risk class is abbreviated by RC.

The process of implementation demands a continuous dialog between physicians and mathematicians since the mathematical modelling requires the determination of numerical constants and functions that cannot be extracted from the rules directly.

The structure of the Fuzzy Inference System reflects the procedure a physician is applying when classifying a thermogram with respect to RC. Roughly speaking the RC is determined by combining several thermogram properties each of them typically involving only a subset of all of the 110 areas. Consequently the expert's interpretation rules can be grouped according to the areas involved, obtaining 13 different groups. In the Expert System this structure is represented by first calculating 13 so-called partial fuzzy values each of them »measuring« the »degree of pathology« of either a single thermogram part or of several thermogram parts with respect to a specific property like for example asymmetry. Afterwards these 13 values are combined using some global rules to obtain the RC. Mathematically the step of computing the partial fuzzy values from the whole thermogram can be understood as a dimension reduction given by a non-linear function  $p: \mathbb{R}^{220} \rightarrow \mathbb{R}^{13}$ .

## 2 Regulation Thermography

Regulation Thermography (RTG) is a diagnostic method in the medical science based on the hypothesis that diseases of the human body (or their prephases) entail characteristic changes in the body's ability to adapt respectively react to the current ambient temperature. Roughly speaking a comparison of the body's actual »thermoregulation ability« with the expected healthy »regulation ability« should give information relevant for the diagnosis of certain diseases.

In this section a brief overview of the physiological basis of RTG is provided. Furthermore, the process of measuring thermograms is described in some detail and necessary terminology is introduced. Finally the »normal« regulation pattern and the basic types of deviations from it are described.

The pictures 1, 2, 3 and 4 are taken from [6].

### 2.1 Physiology of thermoregulation

The healthy body continuously regulates the heat production and loss with the aim to keep up a specific temperature pattern. This pattern is determined by function, anatomy and thermodynamics (figure 1): the temperature of the body's core as well as that of the head must be kept constant as to ensure the unrestricted functioning of the inner organs and the brain. Arms and legs as the other extreme undergo rather strong variation of temperature. The axial symmetry of the temperature distribution has simple anatomic reasons, while the radial decrease of temperature values represents the flow of energy from their source through the body's surface into the ambient space.

The regulation of the heat distribution inside the body is performed by a multitude of components of the human organism forming a complex control system: the center of this system is constituted by the Hypothalamus, a particular part of the brain. Via nerves it is connected to cold and heat receptors distributed

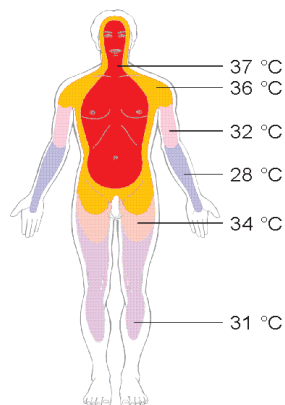


Figure 1: heat distribution

throughout the body and continuously providing a »picture« of the heat distribution. Depending on this picture the Hypothalamus de-/activates the metabolic activity, sends commands to open/close sweat glands or to expand/contract the diameter of blood vessels to mention only a few of the possible regulation mechanisms. Some of these mechanisms are to a certain extent self-sufficient, some others can directly interact with each other. Moreover the communication within the control system is not only conducted via nerves but also via slower chemical channels involving hormones. Altogether the regulation system enables the body to keep its heat distribution constant for ambient temperatures between  $26^{\circ}\text{C}$  and  $32^{\circ}\text{C}$ ; outside this interval deviations from the normal distribution appear. However the organism still keeps functioning properly in a wide temperature range.

To understand in which way a disease can influence the ability for thermoregulation one has to take a look at the body's innervation: neural channels connect the brain with for example inner organs and the skin. Such a channel typically starts in the brain, runs along the spinal cord to a specific point, and leaves the spine between two intervertebral disks to reach its final destination. Due to reasons lying in the embryonal evolution of humans, all nerves leaving the spine between two specific intervertebral disks innervate a »horizontal slice« of the body. The head is an exception from this principle. Moreover the slices might be deformed in vertical direction – see figure 2. The main consequence of this segmentation is that different nerves running to or coming from points in one and the same segment can interact in the spinal cord. An impulse sent by an inner organ can induce an impulse running to a specific part of the skin say. This impulse can alter various properties of the skin, like the temperature, the mechanical tonus and sensitivity, the amount of sweating and so on. The structure just described is called a **reflex arc** and is schematically shown in figure 3. Comprising one can state that pathological changes of an inner organ can locally influence the metabolism, temperature and other properties of the skin via reflex arcs. This fact is the basis of Regulation Thermography.



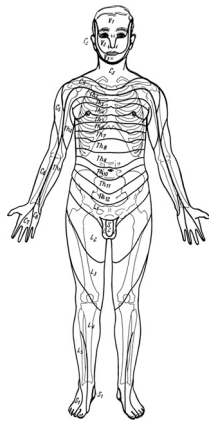


Figure 2: horizontal segmentation

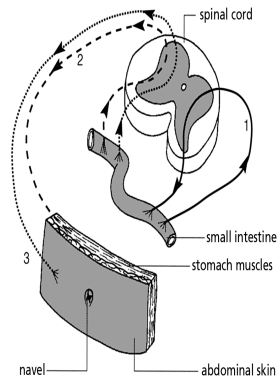


Figure 3: reflex arc

The primary hypothesis of RTG can now roughly be formulated like this:

*An ongoing or emerging disease influences the thermoregulation property of specific areas of the skin in a distinguished way. The knowledge of the abnormally reacting areas combined with a classification of the type of reaction they show in response to a temperature stimulus allows diagnostic conclusions.*

## 2.2 Measurement of the thermoregulation ability

The description of thermoregulation given in the preceding paragraph shows, that the thermoregulation ability cannot be measured *directly* without massive intervention into the body. Instead one investigates the Input-Output behavior of the body's regulation system to judge its status: basically this is done by exposing the proband to a cold stimulus, and measuring the surface temperatures of the body shortly before and a defined amount of time after the onset of the stimulus. Infrared cameras as well as various types of contact thermometers can be used to perform this task. In spite of the advantages of using an infrared camera – it gives a snapshot of the temperature distribution over the whole body and allows the observation of the dynamics of the regulation process – contact thermometers are right now and to our knowledge the preferred method used to retrieve temperatures in RTG. This partially has »historical« reasons, but most likely costs do also play a significant role.

Using a contact thermometer the surface temperature of the body can only be determined at a specified (finite) set of points. In RTG these points are called **areas**, an expression that is used from now on throughout this article. It should however be emphasized that in spite of the misleading name the areas have a well-defined anatomic position. Having fixed a set of areas one measures the body temperature twice at each area: one measurement before and one after the cold stimulus. The set of temperature values so obtained is called a **thermogram**.

To achieve comparability in RTG a standard set of areas was defined by A. Rost in 1975 (see [6]); the thermograms dealt with in the present article are based on this set. It consists of the following members grouped into three subsets:

### The standard areas

The 60 different standard areas are distributed over the whole body in an axial symmetric manner. Since these areas will frequently occur in the subsequent paragraphs, their names and abbreviations are provided in table form below: the areas fall into 8 different subgroups that are shown in the first column of the table. Axial symmetric areas are listed as pairs – like (T1,T2) for the tonsils – occupying only one row in the table. Moreover some areas are grouped together to keep the table short.

The areas at the elbows are measured twice, at the beginning and at the end of each the first *and* the second measurement (E11 equals E13, E12 equals E14). This is done for control purposes: significantly different values at the beginning and the end of a measurement indicate that either the velocity in measuring was too slow or that the regulation equilibrium was not reached yet (second measurement only).

Group	No.	Abbrev.	Name
	1	ST	forehead
	2	NW	root of nose
	3+4	(E11,E12)	elbows
Head	5+6	(SH1,SH2)	frontal sinus
	7+8	(S1,S2)	temples
	9+10	(Aw1,Aw2)	canthus
	11+12	(M1,M2)	mastoids
	13+14	(Sie1,Sie2)	ethmoid bones
	15+16	(KH1,KH2)	maxillary sinus
Throat/ Neck	17+18	(T1,T2)	tonsils
	19-22	L1-4	lymphatic vessels
	23-24	L5-6	supraclavicular fossa
	25-26	L7-8	lymphatic vessels
	27+28	(SD1,SD2)	thyroid gland
Thorax	29	Thy	thymus gland
	30	St	sternum
	31+32	(Mp1,Mp2)	pectoral muscles
	33	He1	atrium/right
	34	He2	atrium/left
	35	He3	cardiac muscle/right
Upper Stomach	36	He4	cardiac muscle/left
	37	Sol	solar plexus
	38	Ma	stomach
	39	Le1	liver
	40	Le3	liver
Intestine	41	Gbl	gallbladder
	42+43	(Pa1,Pa2)	pancreas
	44	Int	intestine
Lower Stomach	45-50	Da1-6	intestine
	51	App	appendix
	52	Ut/Pro	uterus/prostata
	53+54	(Ov1,Ov2)	ovaria
	55+56	(Nie1,Nie2)	kidneys
	57+58	(Isc1,Isc2)	iliosacral joint
	59+60	(E13,E14)	elbows

Table 1: standard areas

**The breast areas**

There are 18 such areas, 9 at each breast, named A1,B1,C1,D1,a1,b1,c1,d1,E1 for the right and with the 1 replaced by 2 accordingly for the left breast. The breast areas are mainly measured for female persons in particular in the context of breast cancer diagnosis.

**The tooth areas**

One such area is located in the face near each of the teeth. The tooth areas play no role in the course of this article.

A rough idea of the location of some of the areas is given by figure 4.

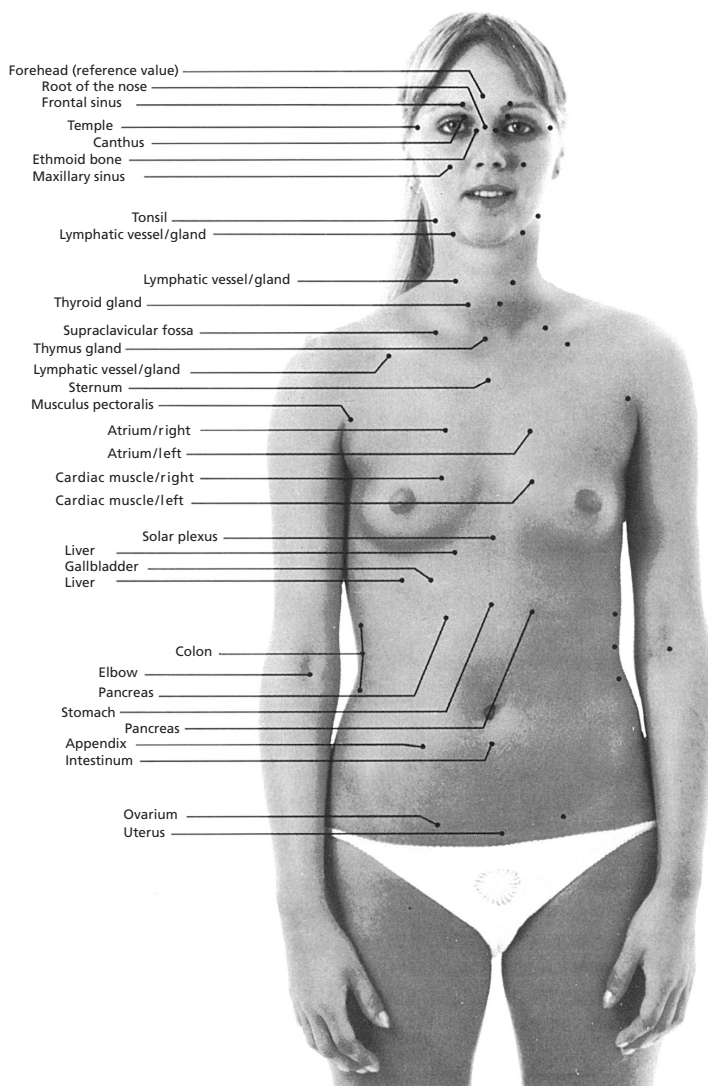


Figure 4: areas at the front of the body

Obviously the process of creating a thermogram needs also to be standardized to produce comparable results: the proband undresses in a room with normed temperature ( $20^{\circ} - 22^{\circ}$  C) and air humidity ( $\sim 60\%$ ) – since the ambient temperature is significantly lower than the mean body temperature a cold stimulus is caused this way. Immediately after undressing the temperatures of the different areas are determined. The measurement should be performed rather quickly to make sure that the onset of thermoregulation does not already influence the temperature values. The measurement is repeated after 20 minutes when the temperature distribution of the body has reached the new equilibrium.

Clearly there are some other points the investigator should care for during the process of thermogram creation. We refer the interested reader to Rost's book [6] for more details.

The totality of 220 values obtained by measuring at Rost's areas twice is called a **regulation thermogram** (RT).

The thermograms evaluated at the ITWM were measured using an electronic preheated thermometer with an adaption time smaller than 0.5 seconds. The temperature values are directly transferred to a Personal Computer and stored together with relevant proband information like age, gender, diseases, ongoing medication etc..

### 2.3 Regulation patterns

In order to quickly gain an overview over the bunch of temperature values a thermogram consists of one frequently used bar plots like the one shown in figure 5: The different areas are listed on the horizontal axis – area abbreviations as well as their numbers are shown – while the vertical axis shows the corresponding temperature values. More precisely bars starting from a line determined by the pre-stimulus-value at the St-area (forehead) depict the pre-stimulus-values in black and the post-stimulus-values in red colour. The St-value normally is not influenced much by stimuli and therefore serves as a **reference line** in the RT.

In figure 5 only the standard areas are shown; they are ordered essentially with respect to their anatomic position from top to bottom. When evaluating an RT the physician has to identify patterns among the temperature values at different areas. Clearly the appearance of a pattern in the bar plot depends on the ordering of the areas. For a human expert it is therefore of importance to always work with one fixed ordering.

For the sake of simplification in the sequel we refer to the pre-stimulus-value of an area A as its **first value** abbreviated by **A(1st)**. The post-stimulus-value consequently is called **second value** and is abbreviated by **A(2nd)**. We shall also use the differences  $A(1st) - St(1st)$  and denote them by **A(temp)**. Finally we are interested in the difference between the second and the first value at the area A. This quantity is called the **regulation at A** and is denoted by **A(reg)**.

Figure 5 demonstrates the normal reaction of the human body to a cold stimulus as well as the expected symmetries. The reader can easily recognize the following overall patterns:

- Areas in symmetric anatomic position have almost equal temperature values. Thus also their regulation almost coincide.

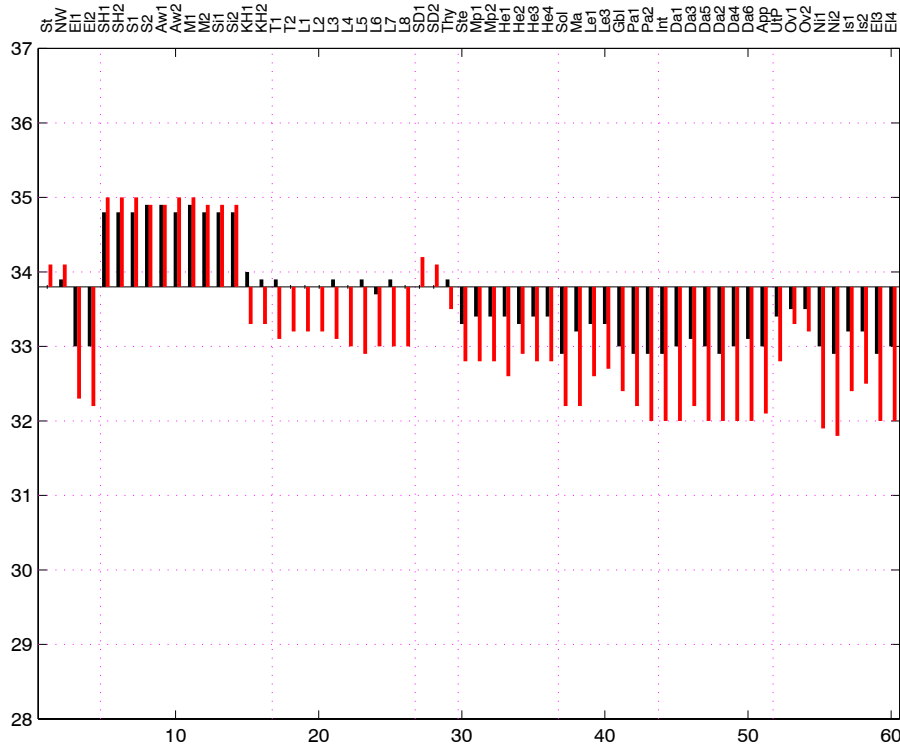


Figure 5: ideal thermogram

- The regulation shows a tendency to increase from top to bottom: while the head areas show only small regulations, the regulation values are around  $-1^{\circ}K$  for the upper and lower stomach areas.
- Most of the regulation values are negative (cold stimulus !) except for the head and the thyroid gland.
- The 1st values of the areas in the thorax, intestine and upper and lower stomach groups are below the reference line.

The reasons for the observed axial symmetry and the top-down pattern visible in the ideal RT are already mentioned in subsection 2.1. As a consequence of the organisms trial to protect the brain against malfunction due to cooling, 1st and 2nd values of the head areas are only slightly differing. At the thyroid gland (areas SD1, SD2) the regulation is positive. As already mentioned one reaction to a cold stimulus is the increase of metabolic activity, a process that involves the hormones produced in the thyroid gland. Therefore increasing metabolic activity yields higher activity of this gland and thus warming up. The distribution of the 1st values about the reference line again mainly has anatomic reasons.

We next take a closer look at the main deviations from normal thermoregulation. Clearly in thermogram interpretation the precise temperature resp. regulation values are used. However in the present subsection we focus on the

qualitative presentation of the most important RT-patterns and postpone a more quantitative description to subsection 3.1.

The »deviations from normality« roughly fall into two classes: local patterns that involve only one area, and patterns that apply to a group of areas or even the whole RT. We start with the explanation of the different

## Local patterns

**Cd-regulation:** the abbreviation »cd« stands for »contra directional« meaning that the sign of the regulation value is the opposite of the expected one. For most of the areas A cd-regulation therefore means  $A(\text{reg}) > 0$ , i.e., as a reaction to the cold stimulus the temperature increases.

An example of cd-regulation can be seen in figure 6 at the areas (Si1,Si2) and at the area UtP. At Si1 and Si2 the regulation values are negative while they should be around zero or slightly positive (head area !). At UtP the regulation value is approximately  $+0.8^\circ K$  but is supposed to be negative.

**Hyporegulation:** regulation having the correct sign but with an absolute value being too small. An example are the areas L1 and L2 in figure 6.

This type of dysregulation seamlessly passes over into

**Rigid regulation:** here no regulation takes place at all although it is supposed to. Typical examples are the areas L7 and L8 in figure 6.

**Hyperregulation:** regulation having the correct sign but with a value being too big. An example is the area Pa2 in figure 7 with a regulation value of approximately  $-2.5^\circ K$ .

**Asymmetry:** deviation from the general rule that anatomically symmetric areas should exhibit almost the same temperature and regulation values independently whether they are normal or pathological. This phenomenon clearly appears at the elbow areas (El1,El2) for both the 1st and 2nd values in figure 6. Moreover the areas (El3,El4) show this behavior too – recall that (El1,El2) equals (El3,El4) and that the values of (El3,El4) are the result of a second measurement at (El1,El2) for control purposes.

**Hotspot:** hotspots are areas with an outstandingly high 1st *and* 2nd value compared to the St-area, where the 1st and 2nd value should show only a small difference.

The local patterns just listed may be qualified further using

## Attributes

As mentioned earlier the temperature values at the areas of a »normal« RT are distributed about the reference value St(1st) in a particular way. While for example the head areas typically display temperatures above the reference line, the values of the torso clearly lie below it. Taking these facts into account pathological patterns may be qualified using the adjectives »hot« and »cold«. Roughly speaking these attributes indicate whether the temperature values involved into the pattern lie above or below the reference line. The exact definition depends on the specific pathology.

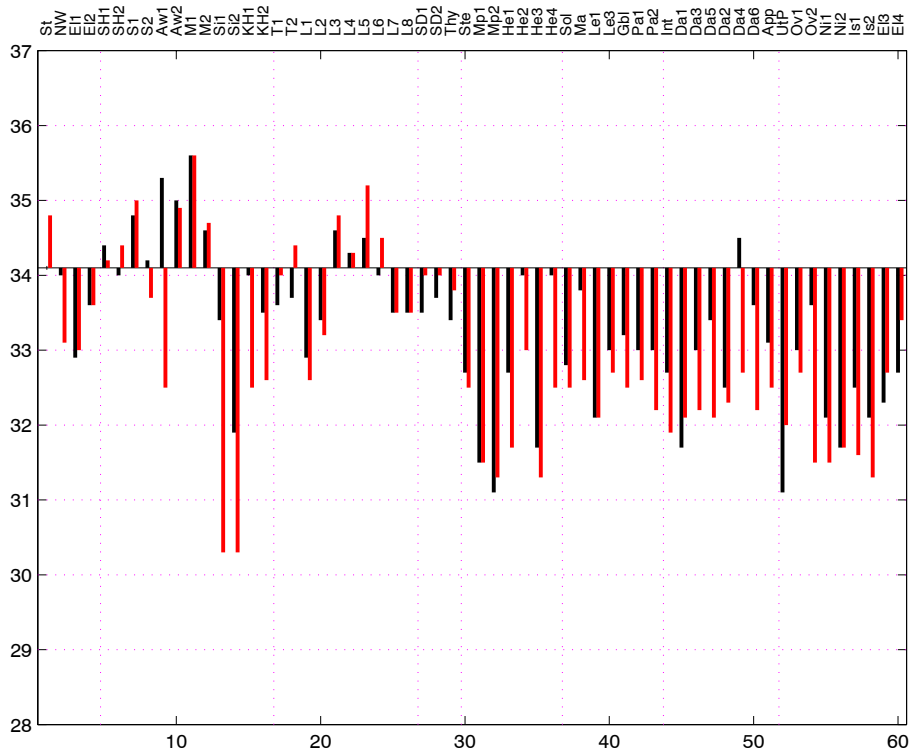


Figure 6: real thermogram, example 1

## Non-local patterns

Beside the behavior of the temperature at isolated areas the experts in Regulation Thermography evaluate the regulation patterns appearing in the area groups as defined in table 1 or even within larger parts of the RT. This represents the fact that an ongoing disease influences several organs each in a specific way. In the sequel we describe some of the more important non-local regulation patterns.

**Regulation type of the RT:** the notions of hypo-,hyper- and rigid regulation do also exist when considering the complete RT instead of only one area. An RT showing hyporegulation for example simply shows hyporegulation at the majority of its areas. The other notions are defined similarly.

**Over-Heating:** this pattern is present in a certain set of areas if the majority of them (usually more than 70%) possess »hot« 1st values, »hot« being understood as an attribute as described earlier in the present section. The RT shown in figure 7 displays over-heating in the upper and lower stomach area group.

**Dissociation:** this rather complex pattern basically consists of a set  $P$  of areas, contained in an area group or a union of anatomically related area groups, with cd- or rigid regulations behaving inhomogeneously with respect to

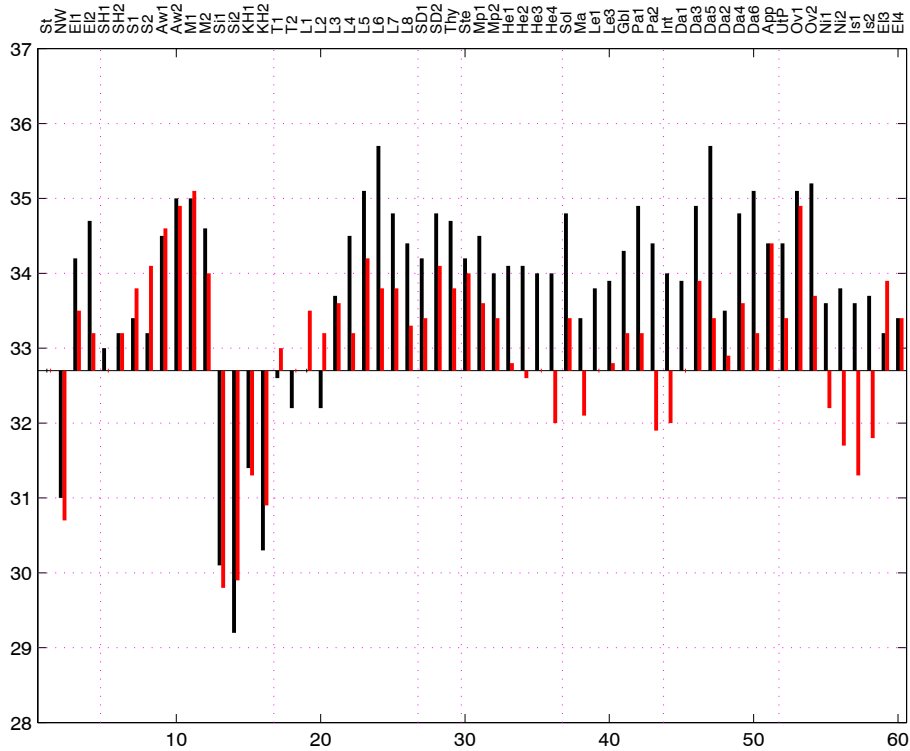


Figure 7: real thermogram, example 2

the attributes »cold« and »hot«: the 1st values of the areas  $A \in P$  are sometimes below and sometimes above the reference value  $St(1st)$ . Moreover ordering the set  $P$  following the anatomy from top to bottom the switching between »cold« and »hot« dysregulations should be nearly alternating.

**Exhaustion:** essentially the exhaustion pattern consists of a set  $P$  of anatomically related areas such that  $A(reg) < c$  for every  $A \in P$ , where  $c < 0$  is a constant typically smaller than  $-1.2^\circ C$ . The set  $P$  can be either a complete area group or a union of such.

A word of warning concerning the terms assigned to the different patterns described in the current subsection: these terms are *not generally used* among the experts applying Regulation Thermography. They are literally translated from the german terms used in the BMBF-project »Datenbasierte Diagnoseunterstützung in der Regulationsthermographie«.



### 3 Regulation Thermography and Fuzzy Logic

The medical interpretation of RTs for diagnostic purposes is based on empiric rules extracted from long-term experience of specialists in the field. These rules are not »sharp« in the sense of a mathematical statement. Rather they do for example depend on only vaguely defined numerical constants or on the visual impression of certain patterns. Furthermore at present there is no commonly accepted set of interpretation rules existing among RTG experts.

In the current section it is shown how Fuzzy Logic can be used to model the expert's thermogram interpretation rules. Furthermore it is explained in which way the so-obtained fuzzy rules in turn can be used as building blocks of an Expert System. Such a system may support physicians in RT evaluation or help them to learn this subject. It can also serve as a database of known interpretation rules and thus help in the process of their critical evaluation.

#### 3.1 Medical interpretation of thermograms

The medical interpretation resp. evaluation of an RT is a complicated process that involves at least the following main steps:

**Analysis of single area groups:** which types of dysregulation occur within an area group and to which extent?

**Combination:** which areas and area groups show significant dysregulation?  
Are there anatomical or functional relationships between the conspicuous areas/area groups existing?

**Global properties:** what is the general tendency of the thermoregulation?  
Are there overall patterns existing in the thermogram?

**Classification:** ... of the RT using some discrete disease-specific classification scheme combining all observed pathologies.

This rough evaluation scheme can of course be refined depending on the particular disease one investigates. Since the authors of the present article are no physicians and do not want to run the risk of providing insufficient or even wrong information the interested reader is once again referred to the source [6]. Instead of stepping into the details of medical RT interpretation we discuss the analysis of single area groups – step 1 in the preceding scheme – utilizing a specific example from breast cancer diagnosis. We also provide an example for the combination process (step 2). However some general remarks about thermogram evaluation should be given beforehand.

Regulation Thermography aims to classify thermograms from a holistic point of view, not so much focussing onto single temperature values. This fact is reflected in the foregoing classification scheme. Consequently it is quite tricky to formulate the evaluation rules precisely, which in turn makes it difficult for newcomers to learn RT-interpretation.

The rules that are presented in the following subsections are quasi-mathematical versions of the rules used by physicians applying Regulation Thermography. They were created in a dialog with such a physician and therefore most likely do not comprehend the full complexity of the »real« rules for at least two reasons: first it is often difficult for a specialist to become aware of the methods utilized

to perform a certain mental classification/evaluation task. Second the dialog between humans working in sciences as different as mathematics and medicine typically suffers from unrecognized misunderstandings. Moreover it is not clear that these rules represent the common sense among the various specialists in RTG. One aim when creating an Expert System for diagnosis support therefore is to provide a tool that helps to fix a common knowledge base.

The evaluation rules themselves partially depend on the kind of disease one wants to investigate. Clearly there is some overlap between the sets of rules for different diseases. For example the lymphatic areas L1-8 are involved in the diagnosis of various types of cancer with similar rules. *In the sequel we are exclusively considering female breast cancer.*

The eventual result of the evaluation of an RT in the situation discussed in this article is a **risk class (RC)** for the presence of breast cancer. Within the BMBF-project mentioned earlier six risk classes numbered from 1 to 6 with increasing risk are used. Thus  $RC = 1$  means that no pathological patterns pointing to breast cancer can be observed in the RT, while  $RC = 6$  expresses the presence of various strongly pronounced breast cancer patterns.

### 3.2 Evaluation of the Thorax group – an example

As an example of the local evaluation rules applied to a single area group we describe the set of rules used to evaluate a part of the Thorax area group. This part consists of the area Sternum (Ste) and the axial symmetric Musculus pectoralis areas (Mp1, Mp2). For reasons of brevity we set  $G := \{\text{Ste}, \text{Mp1}, \text{Mp2}\}$  for this area group.

The rules themselves can be divided into three groups according to the specific qualities of the areas  $A \in G$  they refer to. A fourth set of rules deals with the combination of the observed regulation pathologies.

**Absolute value:** here the differences  $A(\text{temp}) = A(1\text{st}) - \text{St}(1\text{st})$ ,  $A \in G$ , between the 1st temperature values and the 1st temperature value at the St-area (forehead, reference line) are evaluated.

The normal range for each of the three areas is approximately covered by the interval  $[-0.4 \text{ K}, -0.2 \text{ K}]$ . Values above  $+0.2 \text{ K}$  and below  $-0.8 \text{ K}$  are considered as pathological and are referred to as **hot** resp. **cold** areas. The degree of pathology depends on how much the actual value exceeds resp. lies below the given bounds. The maximal degree of pathology is reached at  $+0.6 \text{ K}$  resp.  $-1.2 \text{ K}$ .

**Regulation:** here  $A(\text{reg})$  for  $A \in G$  is taken into account. Again independent of the particular area one has a normal regulation range of  $[-0.8 \text{ K}, -0.5 \text{ K}]$ . Hyper regulation sets in at approximately  $-1.1 \text{ K}$  with an increasing degree of pathology the lower the values are; the maximum is attained at approximately  $-1.4 \text{ K}$ . Rigid and cd-regulation are not treated separately. Instead all values above approximately  $-0.25 \text{ K}$  are classified as deviations from normal behavior, the worst case being values above  $0 \text{ K}$ .

**Asymmetric:** this property involves the values  $1\text{stD} := |\text{Mp1}(1\text{st}) - \text{Mp2}(1\text{st})|$ ,  $2\text{ndD} := |\text{Mp1}(2\text{nd}) - \text{Mp2}(2\text{nd})|$  at the Musculi pectorali discarding the sign of the potential asymmetry. The values of  $1\text{stD}$ ,  $2\text{ndD}$  are supposed to lie below  $0.3 \text{ K}$ , otherwise pathological asymmetry is present depending on

the amount of deviation from normality and reaching the maximal degree at 1.2 K.

**Combination:**

1. The behavior of the three areas  $A \in G$  with respect to their absolute temperatures is summarized in one evaluation treating the areas as follows: if the two Musculus pectoralis areas differ in their behavior only the worst case is taken into the bargain. The evaluation of the area Ste and that of {Mp1,Mp2} are of equal importance. The same procedure applies to the regulation behavior.
2. Pathologies in regulation are considered as being more relevant than pathologies in the absolute temperature values.
3. The total asymmetry in the Musculus pectoralis areas is given by the mean of the asymmetries in the single areas.

Of course the example just presented is rather simple in that it involves only a few areas. In general area groups can be significantly larger than  $G$  as one can see in table 1. Moreover the example does not show the interconnection between the different area groups. However the main principles of RT interpretation are clearly visible already on the presented level.

### 3.3 Fuzzy evaluation rules

In the sequel the representation of RT-interpretation rules in terms of Fuzzy Logic is demonstrated utilizing the example given in subsection 3.2.

All diagrams presented in this subsection were produced using the Fuzzy Logic Toolbox version 2.0 of MATLAB version 5.3, Math Works Inc.

For the convenience of the reader we start by recalling some basic notions of Fuzzy Logic: A **fuzzy set**  $F$  is the graph of a map  $\mu : X \rightarrow [0, 1]$ , i.e.  $F := \{(x, \mu x) \in X \times [0, 1] \mid x \in X\}$ . The set  $X$  frequently is called the **universe** and  $\mu$  is the **membership function of  $F$** . Fuzzy sets occur naturally when modeling properties that are not sharply defined, like for example the property of »being tall« of a human being. In this example the universe  $X$  consists of all human beings and the value  $\mu x$  may be interpreted as the »tallness« of the individual  $x \in X$ . It is frequently useful to think of  $\mu x$  as a »truth value« for a statement made about  $x$ , where  $\mu x = 0$  and  $\mu x = 1$  are interpreted as »false« resp. »true«. The statement itself depends on the fuzzy set  $F$  – in our example it is something like »the person  $x$  is tall«.

The binary variables of Predicate Logic are replaced by so-called **linguistic variables (LVs)** in Fuzzy Logic: a linguistic variable  $V$  takes values in a finite set  $L$ , whose elements are fuzzy sets; these elements are called **linguistic values**. (Remark: the definition of a linguistic variable just presented is a simplified version of the usual one.)

Clearly when replacing binary with linguistic variables one has to redefine the meaning of the basic logical operations »and«, »or«, »negation« and »implies«. If for example  $V_1, V_2$  are linguistic variables and  $L_1, L_2$  possible values of these variables, then the statement » $(V_1 = L_1) \Rightarrow (V_2 = L_2)$ « yields a fuzzy set instead of one of the values »true« or »false«. The method that produces this fuzzy set given the ones of  $L_1$  and  $L_2$  is called the **implication method**. In

contrast to Predicate Logic the implication method as well as the definitions of all other logical operations is not unique but can be chosen subject to certain axiomatic conditions. The choice itself depends on the specific application one has in mind.

The evaluation of a Fuzzy Logic statement typically yields a fuzzy set as a result. On the other hand in applications one wants to get back a single number. This number is derived from the given fuzzy set by application of the **defuzzification method**, which could for example consist of assigning the ordinate of the centroid to a fuzzy set  $A$ .

Finally we have to mention **aggregation** of fuzzy sets: in a system of fuzzy implications the conclusion parts (»right sides«) of the implications yield various fuzzy sets that must be merged or aggregated to obtain the »overall conclusion« of the system – a fuzzy set too. One of the favorite methods to determine the aggregation of fuzzy sets is to take their pointwise maximum.

In order to translate the RT-interpretation rules of subsection 3.2 into Fuzzy Logic we first have to fix a set of linguistic variables sufficient to describe the thermoregulation behavior. In the present case to describe the behavior of the absolute temperature the experts are using the terminology »cold«, »normal« and »hot«, while for the regulation the expressions »hyper«, »normal« and »paradox« apply, where »paradox« regulation comprehends rigid and cd-regulation – see subsection 2.3. We therefore introduce two linguistic variables  $T$  and  $R$  taking values in the sets

$$X_T := \{\text{Cold, Normal, Hot}\} \text{ and } X_R := \{\text{Hyper, Normal, Paradox}\} \quad (1)$$

respectively.  $T$  describes the absolute temperature behavior and  $R$  the regulation. Note that the linguistic value »Normal« can be attained by  $T$  and  $R$ , but this does not necessarily mean that the value »Normal« in both cases is given by the same fuzzy set. From a mathematical point of view we should therefore use different variable names, but for the sake of readability of the fuzzy statements we keep the mathematically ambiguous version.

Next the observed degree of pathology is modelled using the linguistic variables  $P_T$  (absolute temperature) and  $P_R$  (regulation) taking the linguistic values

$$X_{P_T} := \{\text{Negative, Positive}\}, X_{P_R} := \{\text{Negative, Suspicious, Positive}\}. \quad (2)$$

The membership functions of the linguistic values appearing in (1) and (2) are chosen to be trapezoidal: this provides the simplest way to treat those parts of the experts knowledge consisting of critical bounds for temperatures and regulations. The universe of the fuzzy sets in  $X_{P_T}$  and  $X_{P_R}$  are compact intervals – for example the interval  $[-1.5, 0.1] \subset \mathbb{R}$  in the latter case. Once a measurement lies outside the respective interval, it is mapped to the nearest interval border. This procedure reflects the fact that from a medical point of view there is no difference (anymore) between for example a hyperregulation of  $-1.6K$  or a hyperregulation of  $-2.1K$ .

The fuzzy sets in  $X_{P_R}$  are depicted in figure 8.

In terms of Fuzzy Logic the RT-interpretation rules for absolute temperature and regulation at the thorax areas  $A \in G$  now read as follows:

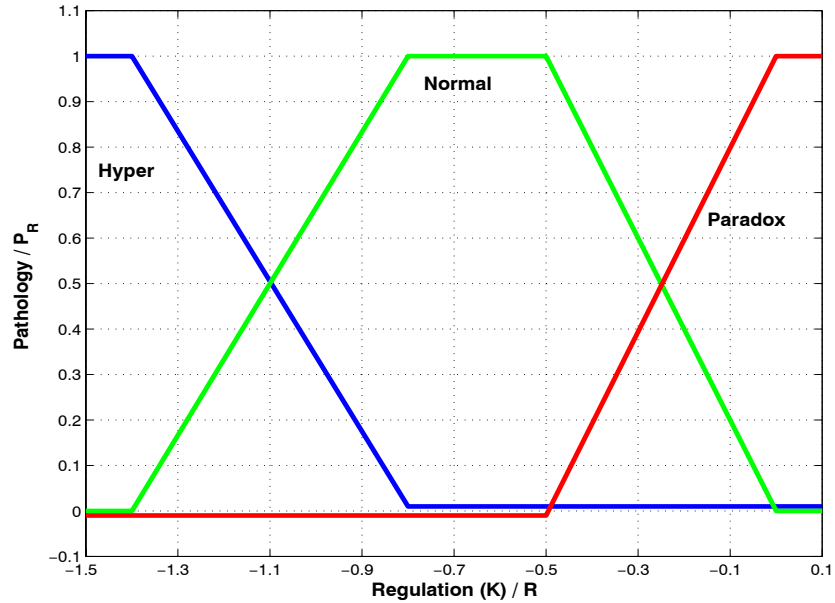


Figure 8: membership functions for the values of  $R$

**Absolute temperature:** If ( $T=Cold$ ) Then ( $P_T=Positive$ )  
 If ( $T=Normal$ ) Then ( $P_T=Negative$ )  
 If ( $T=Hot$ ) Then ( $P_T=Positive$ )

**Regulation:** If ( $R=Hyper$ ) Then ( $P_R=Suspicious$ )  
 If ( $R=Normal$ ) Then ( $P_R=Negative$ )  
 If ( $R=Paradox$ ) Then ( $P_R=Positive$ )

At present no expert knowledge indicates that in the definition of the Fuzzy Logic operators one should deviate from commonly used methods. Therefore the following setting is used:

**Implication:** The membership function of the conclusion is cut off at the fuzzy value corresponding to the input value – so-called minimum method.

**Aggregation:** Maximum of the involved membership functions.

**Defuzzification:** Ordinate of the centroid.

The behavior of a block of rules like for example the one evaluating the regulation observed at an area  $A \in G$  can be represented by graphing the function  $[-1.5, 0.1] \rightarrow [0, 1]$ , that assigns to each regulation value of  $R$  the degree of pathology  $P_R$  determined by aggregating and defuzzifying the fuzzy sets resulting from the three regulation rules. This function is displayed in figure 9.

The rating of asymmetry at the Musculus pectoralis areas Mp1 and Mp2 is performed by evaluating a suitably defined trapezoidal function  $P_A$  at the two observed absolute temperature differences 1stD and 2ndD between the measurements at Mp1 and Mp2. Formally the asymmetry is evaluated using an LV with

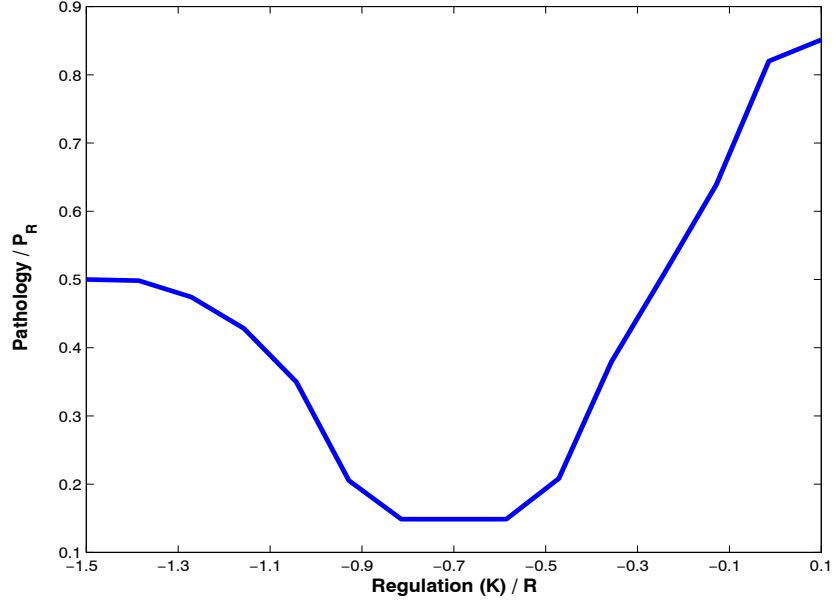


Figure 9: degree of pathology for the regulation

only one linguistic value; consequently the LV and the membership function describing the single value are identified and denoted with  $P_A$ . This function is shown in figure 10.

Eventually we have to determine a method to combine the various evaluation results that we obtain by applying the rules defined so far: the three degrees of pathology  $P_T(\text{Mp1})$ ,  $P_T(\text{Mp2})$ ,  $P_T(\text{Ste})$  for the absolute temperatures, the three degrees of pathology  $P_R(\text{Mp1})$ ,  $P_R(\text{Mp2})$ ,  $P_R(\text{Ste})$  for the regulation, and the degrees of asymmetry  $P_A(\text{1stD})$ ,  $P_A(\text{2ndD})$ . The procedure described in subsection 3.2 to combine these values is brought into the following mathematical form:

$$\begin{aligned}
P_{\text{sternum}} &:= 0.3P_T(\text{Ste}) + 0.7P_R(\text{Ste}) \\
P_{\text{mus.pec.}}^i &:= 0.3P_T(\text{Mpi}) + 0.7P_R(\text{Mpi}), \quad i = 1, 2 \\
P_{\text{asymmetry}} &:= \frac{1}{2}(P_A(\text{1stD}) + P_A(\text{2ndD})) \\
P_{\text{thorax}} &:= \min((P_{\text{sternum}} + \max(P_{\text{mus.pec.}}^1, P_{\text{mus.pec.}}^2) + P_{\text{asymmetry}}), 1),
\end{aligned}$$

where the values  $P_{\text{sternum}}$  and  $P_{\text{mus.pec.}}^i$ ,  $i = 1, 2$ , denote the total scores for the Sternum resp. Musculus pectoralis areas with respect to pathologies of absolute temperatures *and* regulation, while  $P_{\text{asymmetry}}$  is the total score of asymmetry at *both* Musculus pectoralis areas. Eventually  $P_{\text{thorax}}$  is the overall score for the thorax area group. We leave to the reader the task of verifying in detail, that the displayed formulae yield a meaningful model of the combination procedure.

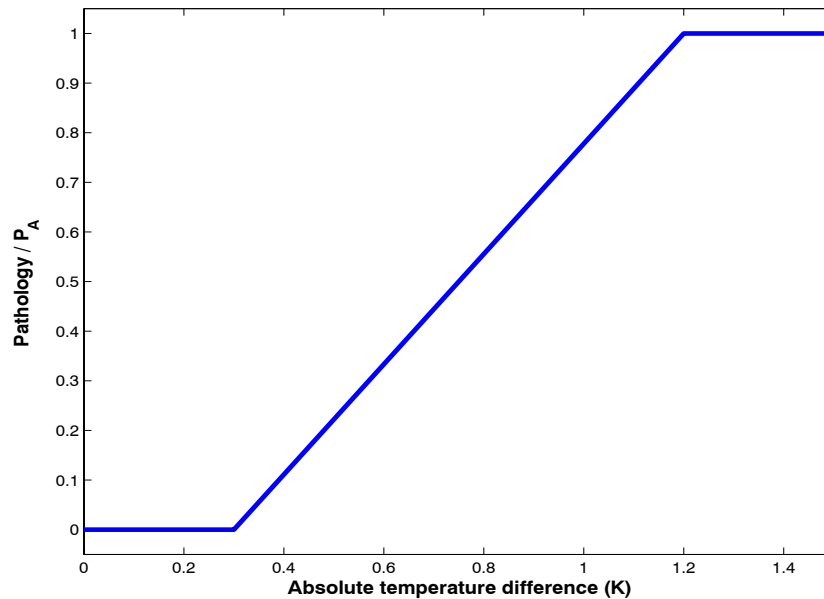


Figure 10: degree of pathology for the asymmetry at Mp1, Mp2

### 3.4 Rudiments of an expert system for diagnosis support

In the subsequent paragraphs an overview is given over the Matlab software package ROST <sup>1</sup> for diagnosis support in Regulation Thermography created by the medical diagnosis group at the department »Adaptive Systems« of the ITWM. The package forms a yet incomplete prototype applicable for the evaluation of regulation thermograms with respect to female breast cancer. Eventually ROST is supposed to contain a complete implementation into Fuzzy Logic of the available expert knowledge in this special field of RT-evaluation.

Matlab in combination with the Fuzzy Logic Toolbox is a convenient »programming language« for quickly building up such a system. As typical for Matlab applications ROST consists of a bundle of Matlab script files (»m-files«) containing the implementation of the functionality; ROST comprises approximately 100 m-files. The technical and structural details of the implementation seem to be of little interest for a reader of this article. Therefore in the subsequent description we focus on the description of ROST's functional components. However for a thorough understanding of these components we have to start our description with some technical facts.

The various components of ROST communicate with each other not only via passing parameters as usual in most programming languages, but also by accessing data that are available in the Matlab workspace of the session from which ROST has been started. The variables containing these data can be considered as global variables, since they are accessible by all m-Scripts. The Matlab work space is initialized immediately after starting ROST and of course its content changes continuously while using the program.

<sup>1</sup>Dr. med. dent. Arno Rost, \*1919, one of the pioneers in Regulation Thermography

ROST consists of four principal functional components; in the sequel we will provide a short description of each of them.

**RT-database:** since ROST currently is not meant to be a tool to evaluate RT's just measured for example in the doctor's practice, it takes the input thermograms from a database. This database not only contains the pure thermogram data (temperature values) but also comprises patient information like gender, age, initial diagnosis, ongoing therapy and progress of the disease resp. healing process. Of course patients *cannot* be identified personally on the basis of these data.

Matlab does not provide real database functionality. The RT-database we are discussing here consists of a Matlab workspace file (»mat-file«) essentially containing the thermogram and patient information in matrix form. The necessary database functionality is implemented in a bundle of m-scripts operating on these matrices once they are loaded into the current (active) Matlab workspace. All scripts can be used standalone, that is in particular independently from ROST itself.

The actual database, that is the thermogram data and patient information, is loaded into the current workspace at startup of ROST.

**Database browser and RT-viewer:** the RT-database can be accessed via a browser that allows to display the information available for a specific thermogram in several ways: on one hand the basic patient information can be shown. On the other hand three different graphical representations of the thermogram itself are available, one of which called the »standard representation« has been used for example in figure 5. The other representations depict the appearing asymmetries in the thermoregulation. Moreover it is possible to restrict the representations to certain area groups instead of the whole thermogram.

**Expert rule database and RT-analyzer:** at the time of writing this article approximately 130 interpretation rules for regulation thermograms with respect to female breast cancer could be formulated in terms of Fuzzy Logic. The Fuzzy Logic Toolbox Version 2.0.1 (R11) was used to implement these rules into an executable Fuzzy Inference System. This system at present consists of approximately 50 files of two types: the files of the first type (»fis-files«) contain the pure Fuzzy Logic components of the evaluation rules broken up into small units (see the subsequent paragraphs). The second group consists of scripts that perform the data pre- and postprocessing as described in subsection 3.3. Some of these scripts moreover control the sequence in which the various components of the Fuzzy Inference System are executed.

The RT-evaluation rules fall into 13 subsets: the rules in such a subset either evaluate a (part of an) area group as defined in table 1 with respect to the overall degree of pathology of the observed thermoregulation behavior, or rate a larger part of the RT with respect to the appearance of certain non-local patterns as roughly described in subsection 2.3. In the sequel the implementation of each of the 13 subsets of RT-evaluation rules is called a **partial RT-evaluation system (PES)**.



Elbows	Elbows
Head	Immunology
Throat/Neck	Tonsils, Supraclavicular fossae, Immunology
T-glands	Thyroid, Immunology
Thorax	Heart, Thorax, Stomach
Upper stomach	Stomach, Dissociation, Immunology
Intestine	Stomach, Dissociation, Immunology
Lower stomach	Ovaria
Mammae	Hotspots, Asymmetry

Table 2: area groups and partial RT-evaluation systems

The sizes of the PESs vary between 7 to 45 rules involving 2 to 25 areas; a typical PES consists of 8 rules and applies to 5 areas. The distribution of the areas within the different PESs can be seen in table 2, where the left column displays the area groups, while in the right column the names of those PESs appear, that refer to areas in the respective group. Among other things one can see from this table that currently only 3 PESs (Stomach, Dissociation, Immunology) are rating non-local patterns. This reflects the fact that complex interpretation rules are not yet completely formalized. The PES »Exhaustion« is not displayed at all due to this incompleteness.

Each of the 13 PESs associates a partial score  $p_i$ ,  $i = 1, \dots, 13$ , to a given thermogram. The  $p_i$  possess a certain medical meaning at least to specialists. The risk class RC for the presence of breast cancer introduced in subsection 3.1 can be considered as a further condensation of these partial scores to obtain a discrete value  $RC \in \{1, \dots, 6\}$ . This condensation is also realized utilizing formalized expert knowledge, but we won't go into the details here.

What we just described is the rough structure of the RT-analyzer, a program that takes thermograms as an input, applies the rules of the PESs to obtain partial scores, condensates the scores to a risk class and yields this class and the partial scores as output.

The Fuzzy Inference System itself can be considered as a database of formalized expert rules: the latter can easily be viewed and edited using the functions of the Fuzzy Logic Toolbox. In combination with the various script files mentioned above we have a system at hand that not only allows to evaluate RTs with respect to the presence of patterns characteristic for female breast cancer, but also enables an expert to critically validate or edit the implemented expert knowledge.

The RT-analyzer is linked to the database browser described previously: it can be started from the browser's user interface and analyzes the thermogram currently loaded by the browser.

**Classification tool:** in the current stage of development ROST is used as a tool in the communication between physicians and mathematicians. During the process of the formalization of expert RT-evaluation rules in terms of Fuzzy Logic it is frequently necessary to adapt numerical parameters like for example temperature thresholds in an appropriate way. To this

end it is useful to have a sufficient quantity of RT's at hand that are classified with respect to RC and the partial evaluation scores by an expert. ROST provides an interface to the RT-database that allows to enter, edit and store these classifications. Like the RT-analyzer this classification tool can be started from the GUI of the database viewer and the data entered refer to the RT currently displayed by the browser.

## 4 Vista

From the medical point of view the principal purpose of research in Regulation Thermography at present lies in a scientific validation of the method, so that it eventually becomes well-accepted among physicians. The expert system ROST is a first step in that direction, since it comprehends the known expert knowledge in the RT-evaluation with respect to breast cancer in an objective manner, which in turn enables scientists to perform comparative tests with the RT-method.

Beside that ROST could also be used in the training of physicians who want to learn about Regulation Thermography.

More concretely within the BMBF-project »Datenbasierte Diagnoseunterstützung in der Regulationsthermographie« several other mathematical methods have been applied in the spirit of the ultimate aim of verification of RT:

- Neural Nets taking the partial scores as an input have been trained to estimate the risk class of a thermogram.
- Support-vector-machines have been used to check whether the medical classification of thermograms can be recovered automatically.
- The method of classification trees has been utilized to extract new RT-evaluation rules from data and discuss them with experts.

It is planned to publish the results obtained with the methods just sketched in forthcoming preprints of the ITWM-series.

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[www.itwm.fraunhofer.de/rd/presse/berichte](http://www.itwm.fraunhofer.de/rd/presse/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. Lentjes, 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 LangmuirHinschelwood 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 nonconvolution 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 noncon-

olution 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 integral modeled viscoelasticity is more general than 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 constraint conditions. This is done by the extension of the Volterra integral operator theory to the Volterra operators with respect to the time, whose 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 originally 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 prescribed 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. To address the specific needs of these users, LoLA was linked 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 tool is embedded in the Advanced Planner and Optimizer SCM software developed by SAP AG, Wall-dorf, 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 multi-criteria 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 Taylor's 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 Mehrskalanalyse 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, Mehrskalanalyse, 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, Poiseuille 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  $\mathbb{R}^3$ , 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, neighborhood 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 satis-

fied 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  $q \in \mathbb{R}^r$  via identification of some of its vertices, a network  $N^\wedge(q)$  is assigned. The paper deals with procedures to find  $N^\wedge(q)$ , such that its determinant  $D^\wedge(s; q)$  admits a factorization in the determinants of appropriate subnetworks, and with the estimation of the deviation of the zeros of  $D^\wedge$  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-Khinchine 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, boundary conditions, 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 efficiency of these storage systems. The presorting task is called Batch PreSorting Problem (BPSP). The BPSP is a variation of an assignment problem, i. e., it has an assignment 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, Assignment, 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 can-

not 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. Mladenović, 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 approxi-

mate 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 that this case can be solved in polynomial time. Offline and online algorithms are presented for solving the BPSP. Competitive analysis is used for comparing the algorithms.

*Keywords: batch presorting problem, online optimization, competitive 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 haystacks", 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 sub-domain. 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. Wirsén

**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 affecting 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 different objects involved in the development process. Based on experimental data, techniques from the field 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 quantification 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)