



**Fraunhofer** Institut  
Techno- und  
Wirtschaftsmathematik

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Towards a Unified Territory Design  
Approach – Applications, Algorithms  
and GIS Integration

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ISSN 1434-9973

Bericht 71 (2005)

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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



# Towards a Unified Territory Design Approach — Applications, Algorithms and GIS Integration

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January 24, 2005

## Abstract

Territory design may be viewed as the problem of grouping small geographic areas into larger geographic clusters called territories in such a way that the latter are acceptable according to relevant planning criteria. In this paper we review the existing literature for applications of territory design problems and solution approaches for solving these types of problems. After identifying features common to all applications we introduce a basic territory design model and present in detail two approaches for solving this model: a classical location–allocation approach combined with optimal split resolution techniques and a newly developed computational geometry based method. We present computational results indicating the efficiency and suitability of the latter method for solving large–scale practical problems in an interactive environment. Furthermore, we discuss extensions to the basic model and its integration into Geographic Information Systems.

*Keywords:* territory design, political districting, sales territory alignment, optimization algorithms, Geographical Information Systems

## 1 Introduction

Territory design may be viewed as the problem of grouping small geographic areas called *basic areas* (e.g. counties, zip code or company trading areas) into larger geographic clusters called *territories* in such a way that the latter are acceptable according to relevant planning criteria. Depending on the context, these criteria can either be economically motivated (e.g. average sales potentials, workload or number of customers) or have a demographic background (e.g. number of inhabitants, voting population). Moreover spatial restrictions (e.g. contiguity,

compactness) are often demanded. We note, that in the literature often the term alignment instead of design is used. As both expressions are interchangeable we will use the latter one throughout this paper.

Territory design problems are motivated by quite different applications ranging from political districting over the design of territories for schools, social facilities, waste collection or emergency services to sales and service territory design. However, the two main applications are political districting and sales and service territory design. In the former application, a governmental area, such as a city or state, has to be partitioned into a given number of territories. As each territory elects a single member to a parliamentary assembly, the main planning criteria is to have approximately the same number of voters in each territory, i.e. territories of similar size, in order to respect the principle of "one man-one vote". The task of designing sales territories is common to all companies which operate a sales force and need to subdivide the market area into regions of responsibility. Closely related to this is the problem of designing service territories for attending to customers or technical facilities. Typical planning requirements are to design territories which are similar in size, e.g. in terms of sales potentials or workload, or which reduce travel times within the territories needed to attend to customers or service incidents.

Due to legal regulations, shifting markets or the introduction of new products, territory design decisions have to be frequently re-evaluated. Especially for a large number of basic areas and territories this is a lengthy task and therefore an algorithmic optimization approach for expediting the process is often desired. For sales territories, well-planned decisions enable an efficient market penetration and lead to decreased costs and improved customer service while in terms of political districting, an algorithmic approach protects against politically motivated manipulations during the territory design process.

When reviewing the literature, one can observe that only few papers consider territory design problems independently from a concrete practical background. Hence the tendency in operations research to separate the model from the application and establish the model itself as a self-contained topic of research can not be observed. However, when taking a closer look at the proposed models for different applications, a lot of similarities can be observed. Indeed, the developed models can often be, more or less directly, carried over to other applications.

Therefore, we will introduce a basic model for territory design and present in detail two approaches for solving the problem: a classical location-allocation approach combined with optimal split resolution techniques and a newly developed computational geometry based method. In the former one, which was already introduced in the mid sixties and has been extensively used since then, the territory design problem is modeled as a discrete capacitated facility location problem and solved by applying a location-allocation method. As territories of similar size are usually obtained in this approach by first solving a continuous, capacitated transportation problem and then rounding the fractional assignments in some non-optimal way in order to obtain non-overlapping territories, we present optimal techniques for resolving the non-integral assignments. Optimal in the sense that the maximal or average deviation of the territory size from the mean is minimal. Since this method is not suitable for the use in an interactive environment, as our computational tests showed, we developed a new method, which is based on computational geometry and utilizes the underlying geographical information of the problem. The idea of this method is to recursively partition the region under consideration geometrically into smaller and smaller subproblems taking the planning criteria into account until an elemental level has been reached where the territory design

problem can efficiently be solved for each of the elemental subproblems. Although the idea for this method was already briefly sketched in the literature, no details were given. We will present computational results indicating the efficiency and suitability of this method for solving large-scale practical problems in an interactive environment.

The rest of the paper is organized as follows. In the next section, we will present various applications for territory design problems found in the literature and identify basic features, common to all applications. Based on these observations we introduce in Section 3 a basic model, which covers most of the previously identified features. In the following section we review the existing literature on models and solution techniques for solving territory design problems and in Sections 5 and 6 present in detail two methods for solving such problems: a classical location-allocation approach combined with optimal split resolution techniques and a newly developed computational geometry based method. In the next section, computational results for the two approaches are presented and in Section 8 we discuss extensions to the basic model and the integration of the presented methods into a Geographic Information System. The paper concludes with a summary and an outlook to future research.

## 2 Applications of territory design problems

In what follows we will present several applications which all have in common the task of subdividing the region under inspection into a number of territories, subject to some side constraints.

### 2.1 Political districting

The problem of determining political territories can be viewed as one of dividing a governmental area, such as a city or a state, into subareas from which political candidates are elected. This problem, usually referred to as *political districting*, is particularly important in democracies where each territory elects a single member to a parliamentary assembly. This is for example the case in Canada, New Zealand, most states in the U.S. and Germany. We note that in this context, territories are usually called *districts*, *census tracks* or *constituencies*.

In general, the process of redistricting has to be periodically undertaken in order to account for population shifts. The length of these periods varies from country to country, e.g. in New Zealand every 5 years, in Canada and the U.S. every decade. To aid this process, operations researchers have developed since the early sixties many different automatic and neutral districting procedures. For recent books on political districting, the reader is referred to Grilli di Cortona et al. [GdCMP<sup>+</sup>99] and Bozkaya et al. [BELN05].

In the past, political districting has often been flawed by manipulation aiming to favor some particular party or to discriminate against social or ethnic minorities. Since the responsibility for approving state and local districting plans usually falls to elected representatives, plans are likely to be shaped implicitly, if not overly, by political considerations, e.g. to keep them in power. A famous case arose in Massachusetts in the early nineteenth century when the state legislature proposed a salamander-shaped electoral district in order to gain electoral advantage. The governor of the state at that time was Elbridge Gerry and this practice became known as gerrymandering. See Lewyn [Lew93] for an interesting description of gerrymandering cases.

To prevent political interference in the districting process, many states have set up a neutral commission, whose functions include the drawing up of political boundaries satisfying a number of legislative and common sense criteria. Depending on the country or jurisdiction involved, these criteria may be enforced by legislative directive, judicial mandate or historical precedent. However, in the scientific literature related to political science, law or geography there is no consensus on which criteria are legitimate for the districting process, i.e. satisfy the neutrality condition. Some are predetermined by constitutional laws, while others are based on common sense and can be disputed. Moreover, it is unclear how they should be measured (Williams [Wil95]). In the following, we will present some of the most commonly used, see e.g. Williams [Wil95], George et al. [GLW97] and Bozkaya et al. [BEL03]. They can be placed under the three general headings: demographic, geographic and political.

### Demographic criteria

**Population equality** When designing electoral districts the main criteria is equity in order to respect the principle of "one man-one vote", i.e. every vote has the same power, and achieve an equitable presence of elected officials. However, depending on the country, deviations from the equal population target are permitted in order to take other criteria into account. Allowed relative deviations from the average range from 5% in New Zealand to 25% in Germany up to, in exceptional cases, 50% in Canada. In the U.S. however, population equality has been deemed by the courts to be very important and as a result the actual deviation now-a-days is in most cases less than 1%.

**Minority representation** The intention of this criterion is to ensure that minority voters have the same opportunity as other members of the electorate to participate in the political process and to elect representatives of their choice (Parker [Par90]). Especially in the U.S., this criteria has become an important consideration during the last 30 years.

### Geographic criteria

**Compactness** A district is said to be geographically compact if it is somewhat round-shaped and undistorted. Although being a very intuitive concept, a rigorous definition of compactness does not exist. Niemi et al. [NGCH90] and Horn et al. [HHV93] propose several measures to assess the compactness of a district, none of which is comprehensive. Compact districts are desired since this reduces the possibility of gerrymandering. In fact, in the U.S., compactness has been defined as simply the absence of gerrymandering. Some authors however argue that the importance of compactness is less than that of other criteria, since gerrymandering is usually not a problem when an algorithm does not use political data (Garfinkel and Nemhauser [GN70]).

**Contiguity** In general, territories have to be geographically connected. First, to protect once more against gerrymandering and second simply because of administrative reasons.

**Boundaries and community integrity** In many cases, districts should be designed such that they adhere to the boundaries of other political constituencies, like cities or counties, or match as closely as possible the boundaries of the previously existing electoral districts. Moreover topological obstacles like mountain-ranges or large bodies of water should be taken into account (George et al. [GLW97]).

## Political criteria

**Political data** Although much disputed some authors decided to consider political data for the redistricting process. For example Bozkaya et al. [BEL03] employ a criteria to achieve socio-economic homogeneity across the districts to ensure a better representation of residents who share common concerns or views. Like Garfinkel and Nemhauser [GN70], they argue that through the use of computer based methods, the possible subjective influence is minimal.

Table 1 provides a selection of articles for political districting problems solved with methods from operations research. It is indicated which of the above mentioned criteria are considered and in addition the country to which the article refers to. Since all authors, without exception, take population equity into account, this criterion is omitted.

Reference	Country	Contiguity	Boundaries	Compactness	Political data
Hess et al. [HWS <sup>+</sup> 65]	USA	+	-	+	-
Garfinkel & Nemh. [GN70]	USA	+	-	+	-
Helbig et al. [HOR72]	USA	+	+	+	-
Bodin [Bod73]	USA	+	-	-	-
Bourjolly et al. [BLR81]	Canada	+	-	+	+
Nygreen [Nyg88]	Wales	+	+	+	-
Hojati [Hoj96]	Canada	-	-	+	-
George et al. [GLW97]	New Zealand	+	+	+	-
Ricca & Simeone [RS97]	Italy	+	+	+	-
Mehrotra et al. [MJN98]	USA	+	+	+	-
Cirincione et al. [CDO00]	USA	+	+	+	+
Bozkaya et al. [BEL03]	Canada	+	+	+	+
Forman and Yue [FY03]	USA	+	+	+	-

Table 1: Selected operations research studies for political districting.

## 2.2 Sales and service territory design

The important but expensive task of designing sales territories is common to all companies which operate a sales force and need to subdivide the market area into regions of responsibility. Closely related is the problem of designing service territories for attending to customers or technical facilities. Here, often quite similar criteria are employed for the design of territories for service staff.

Fleischmann and Paraschis [FP88] report on a German manufacturer of consumer goods who delivers products to several thousand wholesalers. Sales promotions and advertising amongst the retailers is very important in the considered business and is carried out by sales agents, where each agent is in charge of a certain territory. The study was motivated by the impression of the company, that the 8 year old territories seemed to be inappropriate for today's business, mainly because of the uneven distribution of workload. (Hereby, the

workload of a customer was expressed as an internal score taking into account sales value and frequency of visits.)

Blais et al. [BLL03] report on a home-care districting problem in the province of Quebec, Canada. In this case, local community health clinics are responsible for the logistics of home-care visits by health-care personnel, like nurses or physiotherapists, in a given area. If the area is too large, it has to be partitioned into territories, each looked after by a different multi-disciplinary team. Due to a change in the Quebec health care policies, the overall workload increased and became uneven between different territories. To alleviate this problem, the home-care services managers decided to increase their number and re-align them.

In general, there are several motivations for aligning existing or designing new territories. First an increase or decrease in the number of sales- or service-men obviously requires some adjustment of the territories. Other reasons are to achieve better coverage with the existing personnel or to evenly balance workload among the them. Moreover customer shifts or the introduction of new products make it necessary to align territories.

In the following we present several commonly used criteria for sales territory design problems, see e.g. Zoltners and Sinha [ZS83].

### Organizational criteria

**Number of territories** Often, the number of districts to be designed is predetermined by the sales force size designated by the company or planner, see e.g. Fleischmann and Paraschis [FP88]. In case the size is not self-evident, several methods are proposed to compute suitable numbers. For an overview see Howick and Pidd [HP90].

In the past, several authors pointed out, that there exists an interdependency between the sales force size and the territory design and proposed models which assume a variable number of territories, see e.g. Drexler and Haase [DH99].

**Basic areas** Sales territories are in most cases not designed based on single customers. In fact, customers are usually first aggregated into small areas which in turn then serve as a basis for the territory design process. Typical examples for basic areas are counties, zip code areas, predefined prospect clusters or company trading areas. As a result, depending on the level of detail or aggregation, the complexity of the problem reduces considerably and in addition relevant planning data, like sales potentials or distances, is generally much easier to obtain or estimate. Especially the last characteristic has a strong impact on the effort of the planning process.

**Exclusive assignment of basic areas** In most applications basic areas have to be exclusively assigned to a territory. This requirement is motivated by several factors. Most notably, unique allocations result in transparent responsibilities for the sales representatives avoiding contentions among them and allowing for the establishment of long-term customer relations. The latter aspect often goes along with the desire to minimize arbitrary changes in territory boundaries. Moreover, staff-dependent performance reviews are easier to compile.

**Locations of sales representatives** Since sales persons have to visit their territories regularly, their location, e.g. office or residence, is an important factor to be considered in the territory design process. Here, one has to decide whether locations of representatives

are predetermined and should be kept or are subject to the planning process. Zoltners and Sinha [ZS83] remark, that center-seeking territory design approaches have the practical shortcoming, that most sales persons have strong preferences for home-base cities. Fleischmann and Paraschis [FP88] however report in their case study, that management did not want sales persons residences to influence the definition of territories heavily, because addresses can frequently change.

### Geographical criteria

These criteria are mainly motivated by the fact that sales representatives have to travel within their territories.

**Contiguity** Territories should be geographically connected.

**Accessibility** Often a good accessibility of territories, e.g. to highways, or within territories, for example by means of public transportation, is required. Moreover, sometimes non-traversable obstacles like rivers or mountain ranges have to be accounted for.

**Compactness** In most applications, compact territories are an important design criterion. As Hess and Samuels [HS71] point out, one way to improve a salesman's efficiency is to reduce his unproductive travel time. Compact territories usually have geographically concentrated sales (service) activity, therefore less travel, more selling (service) time and hopefully higher sales (better service levels). In other words, the term compactness expresses the desire for territories with minimal total travel times.

In several applications, travel times within territories are in addition considered as part of an activity-related design criterion, e.g. workload. Ronen [Ron83] describes the case of a sales territory design problem for sparse accounts of a distributor in the Midwestern United States, where travel time is even the major design criterion, as the market area of the distributor covers almost five states.

### Activity-related criteria

Geographic requirements on sales territories mainly focus on the travel aspect. However travelling is only a means to an end for the actual work to do, namely selling products or providing service.

**Balance** For sales and service territory alignment problems, often districts which are balanced relative to one or more attributes (called activity measures) are sought for. This criterion expresses a relation of territories among each other and is motivated by the desire of an even treatment of all sales persons. For example in order to evenly distribute workload or travel times among the sales persons or service staff or for reasons of fairness in terms of potential prospects or profit.

Although several different sales territory related attributes have been discussed in the literature (see e.g. Hess and Samuels [HS71], Zoltners and Sinha [ZS83]), one can observe, that only few authors consider more than one criterion simultaneously for designing balanced territories (Deckro [Dec77], Zoltners [Zol79], Zoltners and Sinha [ZS83]).

Apart from the desire for balanced territories, sometimes strict upper or lower bounds for the size of districts are given. For example on maximal travel times or minimal number of customers within the district.

**Maximizing profit** Especially for sales companies, profit is a major aspect in the planning process. Generally a limited resource of call time or effort is available and has to be allocated in a profit-maximizing way amongst a number of sales entities such as customers or prospects. See Howick and Pidd [HP90] for a good overview of commonly used time-effort allocation methods.

To this end, several authors (Lodish [Lod75], Shanker et al. [STZ75], Glaze and Weinberg [GW79], Zoltners and Sinha [ZS83], Skiera and Albers [SA94] and Drexl and Haase [DH99]) propose an integration of time-effort allocation and territory design methods in order to produce more profit and sales than can be obtained by merely using sales potential.

However, Ronen [Ron83] claims, that changing the solution of the strategic territory design problem is much more complicated and expensive than that of the operational time-effort allocation problem and therefore addresses them separately.

Although several methods for integrating time-effort allocation and territory design to maximize profit have been proposed, most procedures still consider the balancing requirement when designing districts. For example to evenly share workload, potential prospects or profit among their sales force. Skiera and Albers [SA94] and Drexl and Haase [DH99], among others, object that the balancing aspect, i.e. fairness or equity, is not the primary criterion for most companies. The main aim should be to maximize profits, regardless of any balancing aspect. Skiera [Ski97] reports of (randomly generated) experiments, where the sales obtained by a pure profit-maximizing approach compared with one taking balance into account, were 5% – 14% higher.

In Table 2 a selection of, in our opinion, important articles for sales and service territory design problems solved with methods from operations research is provided. An extensive overview of models before 1990 can be found in Howick and Pidd [HP90].

For each reference we mark whether a selected criterion is considered in the proposed model ("+") or not ("-"). For the organizational criteria "number of territories" and "locations of sales representatives", a "f" or "v" indicates if the number or locations are fixed or variable. "Mult" stands for models taking more than one activity measure for balance into account. Since the organizational criterion "exclusive allocation" and the geographic "compactness" requirement were considered by all authors without exception, these two are omitted in the table.

## 2.3 Other applications

Besides the most common problems of sales territory design and political districting, several authors report on various other closely related applications.

### 2.3.1 Territories for facilities providing service at a fixed location

In many cases, customers have to visit a (public) facility in order to obtain service, e.g. schools or hospitals.

Reference	Applic.	Organizational		Geographic		Activity-related	
		Nb.	Loc.s	Contig.	Access.	Bal.	Profit
Hess & Samuels [HS71]	Sales/serv.	f	v	-	-	+	-
Easingwood [Eas73]	Service	f	f	+	-	+	-
Shanker et al. [STZ75]	Sales	v	f	+	+	+	+
Segal & Weinberger [SW77]	Service	f	f	+	-	+	-
Glaze & Weinberg [GW79]	Sales	f	v	-	+	-	+
Zoltners [Zol79]	Sales	f	v	+	+	+ / mult	+
Marlin [Mar81]	Service	f	f	-	-	+	-
Ronen [Ron83]	Service	f	f	-	-	+	-
Zoltners & Sinha [ZS83]	Sales	f	f	+	+	mult	-
Fleischmann & Paraschis [FP88]	Sales	f	v	-	v	+	-
Skiera & Albers [SA94]	Sales	f	f	+	+	-	+
Drexel & Haase [DH99]	Sales	v	v	+	+	-	+
Blais et al. [BLL03]	Service	f	-	+	+	-	+

Table 2: Selected operations research studies for sales and service territory design problems.

### School districts

Palermo et al. [PDGT77] and Ferland and Gu nette [FG90] deal with the problem of assigning residential areas to schools. As an outcome of the planning process, all residential areas in the region under consideration are partitioned into a number territories, one for each school. Criteria generally taken into account are capacity limitations on and equal utilization of the schools, maximal or average travel distances for students, good accessibility and racial balance (the latter especially in the U.S.).

### Territories for social facilities

When planning territories for social facilities, like hospitals or public utilities, administrative units have to be aggregated into territories. As a result, it is determined for every inhabitant to which facility he should go in order to obtain service. Typically the number of inhabitants of each territory has to be within predetermined bounds in order to account for a good utilization and a limited capacity of the social facility. Moreover territories should be contiguous and the facilities should be easily accessible for all inhabitants of the respective territory, for example by public transportation. See e.g. Andria et al. [ACP79] and Minciardi et al. [MPZ81].

#### 2.3.2 On-site service territories

Several (public) institutions provide their service not at a fixed location but distributed over a geographic region or on-site where the service incident occurs.

### Winter services and solid waste collection

Muyldermans et al. [MCvOL02] deal with the planning of winter gritting and salt spreading services. On a superior planning level, the region under consideration has to be partitioned into territories, where each territory contains at least one vehicle depot. Afterwards, vehicle

routes for providing service are planned for each territory separately. The main design criteria for the territories are balance, in terms of travel distance, compactness and contiguity. Moreover, territories should allow the planning of "good" routes.

Closely related is the problem of solid waste disposal. In a first step, so-called sectors are determined, where each sector consists of a set of streets or street segments in which waste has to be collected on a certain day. Afterwards, routes for the garbage trucks within the sectors are computed. According to Hanafi et al. [HFV99], the overall time for collecting garbage should be minimized (compactness), the time for collecting garbage should be approximately the same for all sectors (balance) and the sectors should be contiguous.

Whereas in the case study of Muyltermans et al. [MCvOL02], territories are required to be non-overlapping, Hanafi et al. [HFV99] reports that, depending on how often per week waste has to be collected, certain streets can belong to more than one sector, i.e. basic areas are not mutually exclusively assigned to sectors.

### Emergency service territories

D'Amico et al. [DWBR02] report on a case study for police district design, where police departments have to partition their jurisdiction into so-called command districts. After the districts have been fixed, an optimal number of patrol cars that should be on duty is assigned to each command district and the "goodness" of the districts in terms of several different performance measures is assessed. A closely related problem is described by Baker et al. [BCM89], which face the task of designing so-called primary response areas for county ambulances.

As reported, the main design criteria for the territories are workload balance, geographical compactness and contiguity. However, what distinguishes these problems from the previously mentioned is an additional consideration of response times to calls for service, which should be minimized and/or have to be below certain threshold values. These considerations require the incorporation of queueing models and measures: officer or ambulance workloads constitute utilization of servers and response times constitute customer waiting times.

### 2.3.3 Electrical power districting

According to Bergey et al. [BRH03], the World Bank regularly faces the challenge of helping developing countries to move from state owned, monopolistic electric utilities to a more competitive environment with multiple electricity service providers. At that, they face the task of partitioning the physical power grid into economically viable territories (distribution companies). The main aim is to determine territories with approximately equal earning potential in order to provide an environment that will foster competition, and that are compact over a geographic region and therefore easier to manage and more economical to maintain. Moreover, the territories should be non-overlapping and contiguous.

### 2.3.4 Clustering and aggregation of spatial data

Clustering aims at the aggregation of data into classes. On the one hand, each class should comprise data with characteristics as similar as possible and on the other hand, the dissimilarities of data between different classes should be as large as possible. Although the basic task of aggregating smaller units into larger sets is the same for clustering and territory design, the motivations are quite different. The former strives for inner homogeneity of data while

the latter aims at outer similarity. Therefore models for solving both problems are in general not compatible.

However for some aggregation problems, territory design models are applicable. For example Simchi–Levi et al. [SLKSL03] formulate the following guidelines, among others, when aggregating demand points for location problems with the aim of reducing the complexity of the problem: aggregate demand points for 150 to 200 zones; make sure each zone has approximately an equal amount of total demand; place aggregated points at the center of the zone. These guidelines read as a classical center–seeking territory design problem.

### 3 Basic modelling of the territory design problem

Since the early sixties, many authors have investigated territory design problems and provided models for various applications. In the following we will focus on aspects that are shared by most of these models. They cover the essential aspects of territory design problems and can be applied to most of the applications that have been described in the previous section.

Focusing on basic modelling aspects might be considered as a disadvantage, since a user may find that some of his requirements are not reflected in such a model. However, there exist several reasons why general purpose models for territory design are worth studying:

1. Often such a model provides a sufficient approximation for the practical application. For example George et al. [GLW97] and Fleischmann and Paraschis [FP88] report that the solutions obtained by their models were implemented in practice. Both models are rather similar and address the design of electoral districts and sales territories, respectively.
2. The models provide "good" solutions, which can in turn serve as a starting point for manual improvements or local search heuristics, which are able to take more complex criteria into account.
3. There exists a broad range of practical problems to which the models can be applied.
4. General purpose models can serve as a starting point for more complex models that take additional planning criteria into account, depending on the real–world situation.

Our objective is to provide algorithms that run in a general purpose geographical information system. Therefore we do not know the exact problem that a potential user has. Modelling only the most common and basic aspects of the territory design problem allows a wide applicability of the provided algorithms.

In the following we present 'building blocks' for basic models in territory design. Also some notation is introduced that is summarized at the end of this section.

**Basic areas** A territory design problem encompasses a set  $V$  of *basic areas*, sometimes also called sales coverage units. These basic areas are geographical objects in the plane: points (e.g. geo–coded addresses), lines (e.g. street–sections) or geographical areas (e.g. zip–code areas, counties, predefined company trading areas). In the latter case the geographical areas are generally given as polygons. See Figure 1 for an example of basic

areas defined by zip-code regions. In case of non-point objects, a basic area  $v \in V$  is represented by its center with coordinates  $(x_v, y_v)$ .

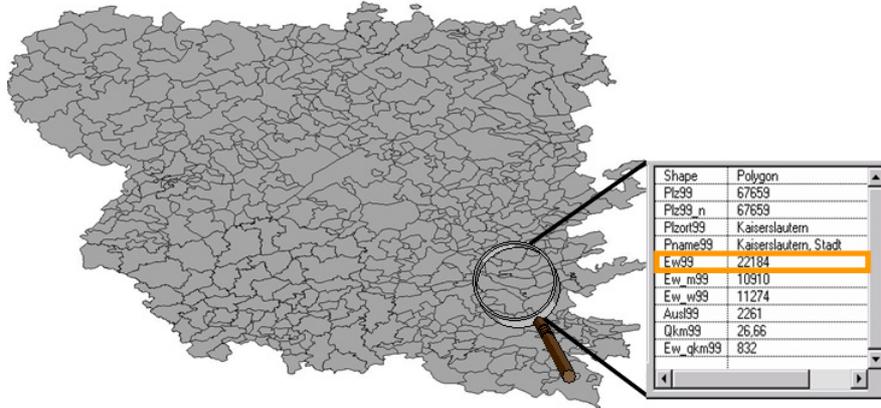


Figure 1: German zip-code areas and associated demographical data. ‘EW’ abbreviates ‘Einwohner’ (inhabitants).

For territory design problems usually one or more quantifiable attributes, called activity measures, are associated with each of the basic areas. Typical examples are workload for servicing or visiting the customers within the area, estimated sales potential or number of inhabitants. See Figure 1 for an example.

We will assume here, that for each basic area  $v \in V$  just a single activity measure  $w_v \in \mathbb{R}_+$  is given. This may also be an aggregation of different values.

**Territory centers** In general, a center is associated with each territory. This may be some specific site, e.g. a salesman residence or office, or simply the geographical center of the territory. In general, the center is identical with the center of one of the basic areas comprising the territory. Therefore, we denote by  $V_c \subset V$  the set of territory centers. In our model these centers can either be predetermined and fixed or subject to planning.

**Number of territories** For the remainder of the paper we assume that the number of territories is given in advance and is denoted by  $p$ . This is not a severe restriction since the algorithms presented below can be adapted to handle the number of territories as a planning parameter.

**Unique assignment of basic areas** We require every basic area to be contained in exactly one territory. Hence, the territories define a partition of the set  $V$  of basic areas. Let  $B_i \subseteq V$  denote the  $i$ -th territory, then

$$B_1 \cup \dots \cup B_p = V \text{ and } B_i \cap B_j = \emptyset, i \neq j.$$

**Balance** All territories should be balanced with respect to the activity measure. Hereby the activity measure (or size) of a territory is the total activity measure of the contained basic areas. Formally,  $w(B_i) = \sum_{v \in B_i} w_v$  is the size of  $B_i$ .

Due to the discrete structure of the problem and the unique assignment assumption, perfectly balanced territories can generally not be accomplished. Therefore a common

way to measure balance is to compute the relative percentage deviation of the district sizes from their average size  $\mu$ . The larger this deviation is, the worse is the balance of the territory.

**Contiguity** In order to obtain contiguous districts, explicit neighborhood information for the basic areas is required. Although there exist several models which are based on a neighborhood graph for the basic areas, we will not incorporate this graph into our considerations. However, the described solution procedures can easily be extended to take a neighborhood graph of the basic areas into account.

**Compactness** We model compactness, depending on the solution method, in two different ways. The first is to minimize the total weighted distance

$$\sum_{i=1}^p \sum_{v \in B_i} w_v d_{iv}$$

(Euclidean, squared Euclidean or network-based) from district centers to basic areas. For the geometric approach we will derive a compactness measure based on convex hulls to achieve compact territories (see Section 6 for details).

**Objective** The objective can be informally described as follows: partition the set  $V$  of basic areas into a number  $p$  of territories which satisfy the specified planning criteria like balance, compactness and contiguity.

To end this section we summarize the notation introduced above.

$V$	set of basic areas
$(x_v, y_v)$	coordinates of $v \in V$
$w_v \in \mathbb{R}_+$	activity measure of $v \in V$
$V_c$	set of territory centers
$p$	number of territories
$B_i \subset V$	$i$ -th territory
$w(B_i)$	size of $B_i$
$\mu = w(V)/p$	average size of territories
$d_{iv}$	distance between $v$ and the center of $B_i$

## 4 Overview of solution techniques

Many territory design approaches have appeared in the literature ranging from location-allocation and set-partitioning methods over divisional algorithms to local search methods and meta heuristics. For extensive reviews, see Howick and Pidd [HP90] and Ricca and Simeone [RS97].

#### 4.1 Location–allocation methods

The first mathematical programming approach was proposed by Hess et al. [HWS<sup>+</sup>65] in 1965 for a center–seeking political districting problem. They modeled the problem as a capacitated  $p$ –median facility location problem. In this problem, we are given a number of already existing facilities (customers) and a number of candidate locations for new facilities. Furthermore, with every customer a demand for a specific product or service is associated which has to be satisfied. Moreover, the new facilities have a limited capacity for satisfying the customer demands. The task is now to locate a certain number of new facilities (e.g. plants, warehouses) among the candidate locations and allocate the already existing facilities to them, taking the capacity of the new facilities into account, such that the demands of the customers are satisfied "efficiently" from or at the new facilities.

Applied to the territory alignment problem, basic areas correspond to customers and their demand to the activity measure attributed to the basic area. Candidate locations for the new facilities are all basic areas. The new facilities to be located are also called *territory centers*. When solving the model, simultaneously new facilities are located among the candidate locations, i.e. the basic areas, and basic areas are allocated to the new facilities, i.e. territory centers. Here, for each territory a center will be located. All the basic areas allocated to the same new facility constitute a territory with the new facility as its center. (Note that this center is not necessarily the geographical center of the territory.) The capacity of the new facilities is chosen in such a way that the districts obtained by solving the problem are well balanced.

Unfortunately, due to its combinatorial complexity, the practical use of this model is fairly limited. To this end, Hess et al. [HWS<sup>+</sup>65] (and subsequently Hess and Samuels [HS71] in their GEOLINE model) used a *location–allocation* heuristic to solve the problem. In this heuristic, the simultaneous location and allocation decisions of the underlying facility location problem are decomposed into two independent phases, a location and an allocation phase, which are iteratively performed until a satisfactory result is obtained. In the location phase the centers of the territories are chosen while in the allocation phase the basic areas are assigned to these centers.

##### Location phase

There exist several approaches for determining a new configuration of territory centers. A fairly simple and commonly used method is to solve in each territory resulting from the last allocation phase a 1–median problem. See e.g. Fleischmann and Paraschis [FP88], George et al. [GLW97]. Alternatively, one can take the territory centers of the previous iteration and perturb them utilizing some local search technique to obtain a new configuration of centers, see e.g. Kalcsics et al. [KMNG02]. Hojati [Hoj96] proposes to determine new centers based on the solution of a Lagrangean subproblem. It shows that the choice of territory centers has a considerable impact on the resulting territories in that a "bad" selection of centers will seldom yield acceptable territories.

##### Allocation phase

In most cases, the problem of allocating basic areas to territory centers is formulated as a capacitated assignment problem, see e.g. Hess et al. [HWS<sup>+</sup>65] and also Section 5. While the balancing requirement is generally included as a side constraint, compact and contiguous

territories are tried to be obtained by minimizing the sum of weighted distances between basic areas and territory centers. For political districting problems, authors tend to use squared Euclidean distances (e.g. Hess et al. [HWS<sup>+</sup>65], Hojati [Hoj96]), whereas for sales territory design problems, largely straight line (Cloonan [Clo72], Marlin [Mar81]) or network distances (Segal and Weinberger [SW77], Zoltners and Sinha [ZS83]) are employed. Marlin [Mar81] observes for his problem, that using squared Euclidean instead of straight line distances produces compact but disconnected territories. He concludes that the success of squared Euclidean distances depends on the ability to redefine territory centers and is not appropriate for the case of fixed centers. A similar phenomenon was observed by Hojati [Hoj96]. Although the model can easily be extended, e.g. to balance more than one activity measure, only those criteria can be incorporated which can be formulated in linear terms. This excludes for example more complex measures of compactness.

The assignment problem now is usually tackled by relaxing the integrality constraints on the assignment variables and solving the resulting capacitated transportation problem using specialized algorithms, like network flow methods, which are suitable for solving large scale problems. Using this approach, George et al. [GLW97] solved a problem with up to 25000 basic areas. However, solving the relaxed problem yields optimal solutions which satisfy the balancing constraints but usually assign portions of basic areas to more than one territory center. To this end, Hess and Samuels [HS71] proposed a simple tie breaking rule, named *AssignMAX*, which exclusively assigns the so-called *split areas* to the territory (center) which "owns" the largest share of the split area. In their applications they found, that a rate, i.e. mean number of areas per territory, of  $n/m \geq 20$  was more than adequate to provide territories whose size was within  $\pm 10\%$  of the average. Fleischmann and Paraschis [FP88], however, report that for their application this simple heuristic gave very poor results. For about 50% of the resulting territories the restriction on the size of the territories was violated, in many cases heavily. (The mean number of areas per territory was approximately 8.) To this end, they presented a more sophisticated split resolution technique which tries to maximize the number of split areas that can be resolved without violating the size restriction on the territories. However, in this way, not all splits could be resolved automatically and some manual postprocessing was required. A quite similar idea to resolve split areas was proposed by Hojati [Hoj96]. Optimal split resolution techniques minimizing the maximal, total or standard deviation from the average are proposed by Schröder [Sch01] and will be discussed in more detail in Section 5.

In order to avoid split areas at all, Zoltners and Sinha [ZS83] propose a slightly different approach. They model the allocation problem as an integer program utilizing so-called SCU-adjacency trees and solve it using Lagrangian relaxation and subgradient optimization.

A completely different allocation approach is to sequentially assign basic areas to territory centers based on distance, i.e. a basic area will be allocated to closest territory center. This minimal distance allocation yields disjoint, compact and often connected, however, usually not well balanced territories as the balance criterion is completely neglected when deciding about the allocation. The attractiveness of this method, denoted as *AllocMinDist*, primarily lies in its simplicity and computational speed. See Kalcsics et al. [KMNG02].

## 4.2 Divisional methods

Among these methods, the *successive dichotomies* strategy of Forrest [For64] and the *wedge-cutting* method of Chance [Cha65] can be mentioned. In the latter case, every district has the shape of a slice of cake and thus touches both the center and the boundary of the region under consideration. However, this approach does not pay much attention to compactness.

Forrest solves the problem by using the principle of diminishing halves. The idea of these types of methods is to iteratively partition the region under consideration into smaller and smaller subproblems, where a subproblem is defined by a set of basic areas and the number of territories, this set has to be partitioned into. The iteration stops if a level has been reached where the territory design problem for each of the subproblems can be solved easily; usually, if the subproblems have to be partitioned just into one territory and therefore already constitute a territory. Hence, given a subproblem, the basic operation is to divide the set of basic areas of the subproblem in a suitable way into two "halves". Unfortunately, Forrest did not provide any details on how he performed this division.

A simple, yet efficient way is to place a straight line in the plane through the set of basic areas of the subproblem, separating it into a right and a left half. The line should be placed in such a way, that the two resulting subproblems are likely to yield contiguous, compact and well balanced territories upon further partitioning. See Section 6 for more details.

## 4.3 Other approaches

Several other methods have been proposed over the past decades, see also Howick and Pidd [HP90] and Ricca and Simeone [RS97].

**Set-partitioning models** Garfinkel and Nemhauser [GN70] proposed a set partitioning based approach to tackle the problem. In a first step, candidate territories are generated which are contiguous, compact and have a total electorate within the tolerance and, in a second step, territories are selected from the set of candidates to optimize the overall balance of the district plan. See also Garfinkel [Gar68].

Mehrotra et al. [MJN98] picked up this model, merely exchanging the objective function by one which minimizes the overall compactness of the territories. They developed a column generation algorithm, which is capable to consider many more potential districts than the initial approach of Garfinkel and Nemhauser and applied it to a districting problem with up to 50 basic areas. Similar approaches are taken by Shanker et al. [STZ75] and Nygreen [Nyg88].

A major advantage compared to location-allocation methods is, that almost any criterion can be applied on the generation of candidate districts. However, due to the combinatorial complexity, set-partitioning models have not been used with more than 100 basic areas.

**Criteria methods** These are manual approaches, which provide sales management with data and an objective for sales territory alignment, but do not provide a methodology for actually designing the territories. See e.g. Easingwood [Eas73], Lodish [Lod75].

**Eat-up** In this approach, one territory after the other is extended at its boundary through successively adding yet unassigned, adjacent basic areas to the district, until it is sufficiently large. See e.g. Mehrotra et al. [MJN98].

**Clustering** Deckro [Dec77] proposed an approach, where each basic area is initially treated as a single district. Then iteratively pairs of districts are merged together forming new and bigger territories until the prescribed number of districts is reached.

**Multi-kernel growth** This method starts by selecting a certain number of basic areas as "seeds" (centers) for the districts. The algorithm then successively adds to each center neighboring basic areas, in order of decreasing distance, until the desired territory size is reached. See e.g. Bodin [Bod73].

**Local search** The well known local search techniques are heuristic methods, which try to improve an existing territory plan by successively shifting basic areas between neighboring territories with the aim of minimizing a weighted additive function of different planning criteria.

A simple approach is employed by Bourjolly et al. [BLR81]. More sophisticated algorithms based on simulated annealing are proposed by Browdy [Bro90], Macmillan and Pierce [MP92] and D'Amico et al. [DWBR02]. Ricca [Ric96] develops descent, simulated annealing and tabu search algorithms. The latter technique has been successfully applied in the recent papers of Bozkaya et al. [BEL03] and Blais et al. [BLL03]. See also the upcoming book of Bozkaya et al. [BELN05].

**Genetic algorithms** Genetic algorithms for solving territory design problems have been introduced recently by Forman and Yue [FY03] and Bergey et al. [BRH03]. The former authors utilize a technique based on an encoding and on genetic operators used to solve Traveling Salesman Problems. The encoding chosen is a path representation and a single chromosome travels through each basic area, and as the areas are traversed, territories are formed by the sequence of basic areas. Bergey et al. [BRH03] use their own representation and, moreover, incorporate a simulated annealing method to improve results.

## 5 A location-allocation method with optimal split resolution

Hess et al. (1965) [HWS<sup>+</sup>65] were the first to model the problem of designing political districts as a mixed integer linear program. Essentially the model is discrete capacitated facility location problem.

Trying to solve this  $\mathcal{NP}$ -hard MIP with a commercial solver was not possible at the time of the paper of Hess et al. and is today still not suitable for a decision support system in an interactive environment. The reason is that the running time of the solver to find an optimal solution and to prove its optimality depends in a non-predictable way on the problem data. The user in the interactive environment on the other hand will not accept such a behavior of his software tool.

Therefore to solve their MIP in a heuristic fashion, Hess et al. use a location-allocation procedure. In the location phase the centers of the districts are chosen while in the allocation phase the basic areas are assigned to these centers. The location part is simple, in each territory resulting from the last allocation phase a 1-median problem is solved.

Here we are concerned mainly with the allocation phase. In the following we will discuss how Hess et al. solve it and present a technique for optimal split resolution. The material in this section is taken from Schröder (2001) [Sch01].

### 5.1 The allocation problem

Let  $V$  be the set of basic areas and  $V_c \subset V$  the set of  $p$  territory centers. For  $v \in V$  and  $i \in V_c$  let  $d_{iv}$  be the distance from  $i$  to  $v$ . The average territory size is  $\mu = w(V)/p$ . Let  $\tau > 0$  be a tolerance value for the deviation of the actual sizes of the territories from  $\mu$ .

With the assignment variables

$$x_{iv} = \begin{cases} 1 & \text{if basic area } v \text{ is assigned to center } i \\ 0 & \text{otherwise} \end{cases}$$

Hess et al. (1965) [HWS<sup>+</sup>65] proposed the following allocation model:

$$(ALLOC) \quad \min \quad \sum_{v \in V} \sum_{i \in V_c} w_v d_{iv} x_{iv}$$

$$\text{s.t.} \quad \sum_{i \in V_c} x_{iv} = 1 \quad \forall v \in V \quad (1)$$

$$(1 - \tau)\mu \leq \sum_{v \in V} w_v x_{iv} \leq (1 + \tau)\mu \quad \forall i \in V_c \quad (2)$$

$$x_{iv} \in \{0, 1\} \quad \forall v \in V, i \in V_c \quad (3)$$

The objective function minimizes the overall distance, weighted with the activity measure, from the basic areas to the respective territory centers. The model tends to produce compact and also geographically connected territories. Constraints (1) ensure that each basic area is allocated to exactly one territory center (disjointness criterion). By (2) we enforce that the size of each of the territories is within the predefined tolerance (balance criterion). In total we have a quadratic number of decision variables and a linear number of constraints.

The outcome of the model depends a great deal on the parameter  $\tau$ . The smaller the tolerance  $\tau$  is the better the balance of the obtained territories. Unfortunately, if  $\tau$  is too small, i.e. the upper and lower bounds on the size of the districts in constraints (2) are very tight, then territories tend to be no longer compact and connected; the problem might even become infeasible. In addition the complexity of the problem and therefore the time for solving it generally increases the smaller  $\tau$  is. On the other hand the larger the tolerance is the worse the balance of the territories will be.

The way of Hess et al. to overcome this problem is as follows. They set the tolerance to  $\tau = 0$  and relax the integrality constraint on the assignment variables  $x_{iv} : x_{iv} \in [0, 1]$ . Then  $x_{iv}$  is the fraction of basic area  $v$  allocated to territory center  $i$ .

This relaxed problem is a linear program which is basically a classical transportation

problem.

$$(TRANSP) \quad \min \quad \sum_{v \in V} \sum_{i \in V_c} w_v d_{iv} x_{iv}$$

$$\text{s.t.} \quad \sum_{i \in V_c} x_{iv} = 1 \quad \forall v \in V \quad (4)$$

$$\sum_{v \in V} w_v x_{iv} = \mu \quad \forall i \in V_c \quad (5)$$

$$x_{iv} \geq 0 \quad \forall v \in V, i \in V_c \quad (6)$$

Problem TRANSP can efficiently be solved using specialized network algorithms. In the optimal solution of TRANSP the territories are perfectly balanced. On the other hand the criterion of disjointness is generally not satisfied, due to the continuous variables in TRANSP. A basic area  $v$  for which more than one variable  $x_{iv}$ ,  $i \in V_c$  has positive values is called *split area* or just *split*. For a basic (optimal) solution of TRANSP it is easy to prove that there are at most  $p - 1$  splits.

To establish the criterion of disjointness after the solution of TRANSP it is necessary to round for every split its fractional variables to one (one variable) or zero (the other variables). This yields disjoint territories but on the other hand destroys their perfect balance. Since there are many possibilities for the rounding, we want to find one that results in as much as possible balanced territories. We call this the *split resolution problem*.

## 5.2 The split resolution problem

Let  $V^S \subset V$  be the set of splits in the optimal solution of TRANSP. We want to resolve the splits while keeping the territories as balanced as possible. To quantify this objective we have different possibilities:

- (SPRES<sub>∞</sub>) Minimize  $\max\{|W_i - \mu| : i \in V_c\}$  (maximum deviation)
- (SPRES<sub>1</sub>) Minimize  $\sum(|W_i - \mu| : i \in V_c)$  (total deviation)
- (SPRES<sub>2</sub>) Minimize  $\sum((W_i - \mu)^2 : i \in V_c)$  (equiv. to standard deviation)

where  $W_i = w(B_i)$  is the size of the territory with center  $i$ .

To further examine the problem of split resolution we need a definition, given first by Fleischmann and Paraschis [FP88]: Let  $(x_{iv})$  be an optimal basic solution of TRANSP. The graph  $T^S = (U^S, E^S)$  with  $U^S = V_c \cup V^S$  and  $E^S = \{(i, v) : 0 < x_{iv} < 1\}$  is called *split adjacency*. The edges of the split adjacency correspond to the fractional variables in the solution  $(x_{iv})$  of TRANSP. Clearly,  $T^S$  is cycle-free, i.e. a forest. Figure 2 visualizes the definition of the split adjacency.

In Hess and Samuels [HS71] and also in George et al. [GLW97] a simple rule is proposed for split resolution: They assign every split  $v$  fully to the center  $i$  for which  $x_{iv}$  is maximum. Schröder [Sch01] calls this heuristic for resolving the splits *AssignMAX*.

In Schröder [Sch01, p.147] it is proven that AssignMAX has no finite guarantee for minimizing the maximum deviation (i.e. problem SPRES<sub>∞</sub>). An example is given in which the maximum deviation resulting from AssignMAX grows as  $d^2 - d$ , while it is possible to resolve the splits in a way that yields a maximum deviation of  $2d$ . Here  $d \geq 4$  is the maximum node degree in the split adjacency used in the example.

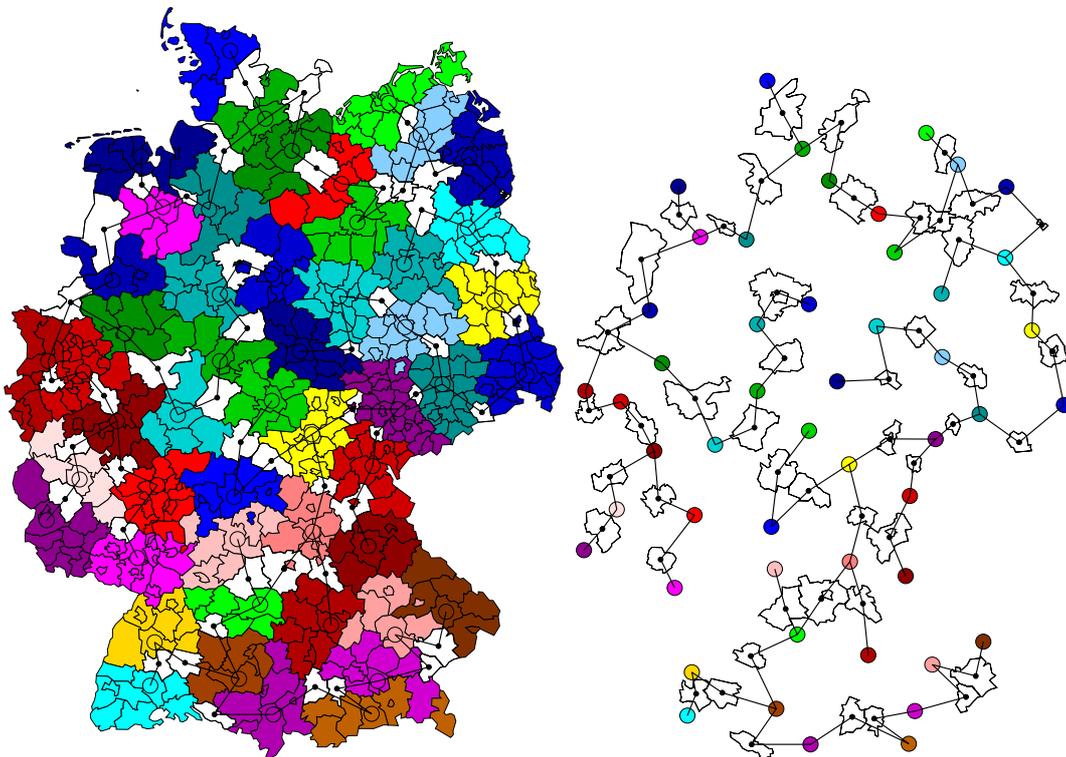


Figure 2: Left: structure of the optimal solution of TRANSP. The edges shown correspond to fractional variables. Right: the corresponding split adjacency.

This result is more of theoretical interest since in split resolution problems coming from real world data we can assume that the degrees of the nodes in the split adjacency are not very large. The following theorem gives an upper bound on the maximum deviation of the territory sizes from  $\mu$  in terms of the degrees in the split adjacency.

**Theorem 1** *Let  $\bar{\delta}_V = \max\{\deg(v) : v \in V^S\}$ ,  $\bar{\delta}_I = \max\{\deg(i) : i \in V_c\}$  (degrees in  $T^S$ ) and  $\bar{w} = \max\{w_v : v \in V^S\}$ . Then*

$$\max\{|W_i - \mu| : i \in V_c\} \leq (1 - 1/\bar{\delta}_V)\bar{\delta}_I\bar{w},$$

where  $W_i$  is the size of the territory with center  $i$  after the application of AssignMAX.

*Proof.* For a given  $v \in V^S$  let  $i \in V_c$  be the center to which  $v$  is assigned by AssignMAX. By the definition of this heuristic

$$x_{iv} = \max\{x_{i'v} : i' \in V_c, x_{i'v} > 0\}.$$

The number of positive  $x_{i'v}$ ,  $i' \in V_c$  is equal to  $\deg(v)$  in  $T^S$ . Therefore  $x_{iv} \geq 1/\deg(v)$  and by assigning  $v$  to  $i$  the size of the territory with center  $i$  increases by at most  $w_v(1 - 1/\deg(v))$ . It follows that the maximum size of a territory is at most  $(1 - 1/\bar{\delta}_V)\bar{\delta}_I\bar{w}$  larger than  $\mu$ .

If on the other hand a split  $v$  is not assigned to center  $i$  then  $x_{iv} \leq 0.5$ . Consequently the minimum size of a territory is at most  $(1/2)\bar{\delta}_I\bar{w}$  smaller than  $\mu$ . Since  $\bar{\delta}_V \geq 2$  this is bounded by  $(1 - 1/\bar{\delta}_V)\bar{\delta}_I\bar{w}$ .  $\square$

### 5.3 Optimal split resolution

Solving the problem of split resolution in an optimal fashion means that we solve one of the problems  $\text{SPRES}_1$ ,  $\text{SPRES}_2$  and  $\text{SPRES}_\infty$  to optimality. The following result, proved in [Sch01], shows the computational complexity of these problems.

**Theorem 2**  *$\text{SPRES}_1$  and  $\text{SPRES}_2$  are  $\mathcal{NP}$ -hard, while  $\text{SPRES}_\infty$  can be solved polynomially.*

This result assumes that the degrees in the split adjacency can become arbitrarily large. If we assume that in practical problems the maximum degree in  $T^S$  is bounded, the algorithm we present next for the optimal solution of the split resolution problem runs in linear time. This algorithm is generic and solves  $\text{SPRES}_*$ , where  $*$  is one of  $1, 2, \infty$ .

Our algorithm for optimal split resolution is a dynamic programming procedure and is based on the absence of cycles in the split adjacency. W.l.o.g we can assume that the split adjacency  $T^S$  is a tree (otherwise we insert some arbitrarily chosen edges into the forest until it is connected). Further we select some node  $v_0 \in V_c$  and consider  $T^S$  as a rooted tree with root  $v_0$ .

The procedure works in  $T^S$  from the leaves to the root and computes the optimal value of the selected objective function. Thereby it makes use of the fact that there are two different types of nodes in  $T^S$  corresponding to splits and territory centers. Every edge in  $T^S$  joins two nodes of different type.

The process of split resolution is equivalent to the solution of a tree partitioning problem for the split adjacency: partition  $T^S$  into subtrees that contain exactly one node from  $V_c$ . More precisely the node set  $U^S$  is partitioned into subsets that induce a subtree of  $T^S$  and have a one-element intersection with  $V_c$ .

To proceed we need some notation. Let  $T' = (U', E')$  be a subtree of  $T^S$ .  $T'$  is feasible if  $|U' \cap V_c| = 1$ . We associate a cost with  $T'$ , depending on the selected objective function:

$$c(T') := c(U') := \begin{cases} |w(U') - \mu| & \text{for SPRES}_1 \text{ and SPRES}_\infty \\ |w(U') - \mu|^2 & \text{for SPRES}_2 \end{cases}$$

The cost measures the deviation of the weight of the subtree from the average weight. Here we define the weight of a node  $i \in V_c$  corresponding to a center as the total weight of this node and all uniquely assigned nodes  $v$  in  $V$ , i.e. with  $x_{iv} = 1$ .

Since we are searching for the optimal partition of  $T^S$  into feasible subtrees, we define the cost of a partition  $\pi = \{T'_i : i \in V_c\}$  as a generalized sum of the cost of the subtrees

$$c(\pi) = \bigoplus_{i \in V_c} c(T'_i)$$

where

$$\oplus = \begin{cases} + & \text{for SPRES}_1 \text{ and SPRES}_2 \\ \max & \text{for SPRES}_\infty \end{cases}$$

A partition  $\pi$  of minimal cost corresponds to a split resolution with most balanced territories, where the deviation is measured by the selected objective function  $\text{SPRES}_*$ .

We introduce some further notation related to the rooted tree  $T^S$ . For  $u \in U^S$  let  $T_u$  denote the subtree rooted in  $u$ , i.e. the subtree containing  $u$  and all its descendants.  $\text{pre}(u)$  is the father of  $u$  and  $S_u$  is the set of sons of  $u$ .

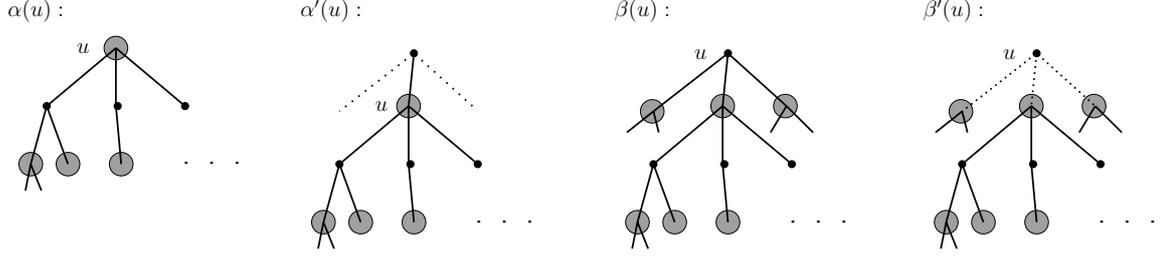


Figure 3: Partial optima in the dynamic programming procedure for the partitioning of  $T^S$ . Circles depict center nodes, dots are split nodes.

In the recursion of the dynamic programming procedure we denote the optimal value of the objective function for different partial problems in the following way (see Figure 3).

- For  $u \in V_c$ ,  $\alpha(u)$  is the cost of an optimal partition of  $T_u$ .
- For  $u \in V_c$ ,  $\alpha'(u)$  is the cost of an optimal partition of  $T_u \cup \{\text{pre}(u)\}$ .
- For  $u \in V^S$ ,  $\beta(u)$  is the cost of an optimal partition of  $T_u$ .
- For  $u \in V^S$ ,  $\beta'(u)$  is the cost of an optimal partition of the forest  $T_u - \{u\}$ .

To work from the leaves to the root in  $T^S$  we use the following recursions. If  $u$  is a leaf then  $u \in V_c$  (since all nodes corresponding to splits have degree  $\geq 2$  in  $T^S$ ) and

$$\alpha(u) = c(\{u\}) \quad \alpha'(u) = c(\{u, \text{pre}(u)\}).$$

If  $u \in V^c$  is not a leaf

$$\alpha(u) = \min_{S' \subseteq S_u} \left\{ c(\{u\} \cup S') \oplus \bigoplus_{u' \in S'} \beta'(u') \oplus \bigoplus_{u' \in S_u - S'} \beta(u') \right\} \quad (7)$$

$$\alpha'(u) = \min_{S' \subseteq S_u} \left\{ c(\{u, \text{pre}(u)\} \cup S') \oplus \bigoplus_{u' \in S'} \beta'(u') \oplus \bigoplus_{u' \in S_u - S'} \beta(u') \right\} \quad (8)$$

Here  $S'$  denotes the set of sons that are included in the subtree for the center node  $u$ .

If  $u \in V^S$

$$\beta(u) = \min_{u' \in S_u} \left\{ \alpha'(u') \oplus \bigoplus_{u'' \in S_u - \{u'\}} \alpha(u'') \right\} \quad (9)$$

$$\beta'(u) = \bigoplus_{u' \in S_u} \alpha(u') \quad (10)$$

The verification of (7) to (10) is straightforward. Since nodes of center type and nodes of split type alternate in  $T^S$  equations (7) to (10) can be applied recursively until finally  $\alpha(v_0)$  is found. This is the cost of an optimal partition. This partition (and hence the optimal split resolution) can then be determined by backwards calculation.

The calculation of  $\alpha(u)$  and  $\alpha'(u)$  according to (7) and (8) generally requires exponential time, whereas the calculation of  $\beta(u)$  and  $\beta'(u)$  (equations (9) and (10)) can be done in linear time. In summary we find:

**Theorem 3** *An optimal split resolution can be computed in  $O(\bar{\delta}_I 2^{\bar{\delta}_I} |V_c| + \bar{\delta}_V |V^S|)$  steps.*

For bounded maximum degree in the split adjacency this is linear. Note that also AssignMAX requires linear time. For problem SPRES $_{\infty}$  the optimization problems (7) and (8) can be solved in polynomial time, regardless of the degree of nodes in  $T^S$ . More precisely the following theorem is proved in Schröder [Sch01].

**Theorem 4** *SPRES $_{\infty}$  can be solved in  $O(\bar{\delta}_I^3 |V_c|^2 \log \bar{w} + \bar{\delta}_V |V^S|)$  steps.*

Equations (7) to (10) yield also a better worst case estimate for SPRES $_{\infty}$  than AssignMAX (cf. Theorem 1).

**Theorem 5** *Let  $\bar{w} = \max\{w_v : v \in V^S\}$ . For the optimal solution of SPRES $_{\infty}$  we have*

$$\max\{|W_i - \mu| : i \in V_c\} \leq \bar{w},$$

where  $W_i$  is the size of the territory with center  $i$ .

The proof is not difficult and works by showing that for all  $u \in U^S$   $\alpha(u), \alpha'(u) \leq \bar{w}$  and  $\beta(u), \beta'(u) \leq \bar{w}$ , respectively. This can be done by induction using equations (7)–(10) written down for the case of SPRES $_{\infty}$ . See [Sch01, p.161] for details.

#### 5.4 The location phase

The allocation method proposed in the preceding section can be combined with any method to determine good territory centers. Approaches for this task have been shortly described in Section 4.1. We refer to the literature cited there for more information on the location phase.

#### 5.5 Comment on the location-allocation method

The location-allocation method has the advantage that the solution of the MIP ALLOC is not required. Instead in each iteration the linear program TRANSP has to be solved. This can be done rather efficiently. However we found that the running time is still too high for the solution of large-scale problems with many thousands of basic areas in an interactive environment.

We can make the allocation step much faster by assigning every basic area to the nearest center. This means that we drop constraints (2). This *AllocMinDist* heuristic has a greatly reduced running time. However, as one would expect and as the computational results in Section 7 show, the balance of the territories obtained is not satisfactory.

Therefore in the next section we present a new heuristic based on geometric ideas. It has the desirable property of being very fast (comparable to location-allocation with *AllocMinDist*) and producing territories that are balanced comparable to location-allocation with TRANSP and split resolution with AssignMAX.

## 6 A computational geometry based heuristic

Although the idea of using methods of computational geometry has already been mentioned in the literature, Forrest [For64], no details were given.

The idea of the method presented here is to recursively partition the complete problem geometrically using lines into smaller subproblems until an elemental level is reached where we can efficiently solve the territory design problem for each of the elemental subproblems. The solutions to these problems then directly yield a solution for the original problem.

A territory is given by a subset  $B$  of  $V$ . The heuristic strives to align territories that are balanced with respect to the activity measure. Ideally we would have  $w(B) = w(V)/p$  for every district, but in general this is not possible due to the discrete nature of the problem. Therefore we assume that a lower bound  $L$  and an upper bound  $U$  for the activity measure of a territory are given. For example,  $L$  and  $U$  can be calculated from a maximally allowed deviation  $\tau > 0$  from average size by

$$L = (1 - \tau)w(V)/p \quad \text{and} \quad U = (1 + \tau)w(V)/p. \quad (11)$$

A territory  $B$  is called *feasible* if  $L \leq w(B) \leq U$ .

In the following we will often identify (sets of) basic areas with (sets of) points in the plane.

### 6.1 Main ideas of the heuristic

The basic operation of this heuristic is to divide a subset  $V' \subseteq V$  of the basic areas, i.e. points, into two "halves"  $V'_l$  and  $V'_r$  by placing a line in the plane within this set of points.  $V'_l$  ( $V'_r$ ) are then defined as the set of points, i.e. basic areas, located left (right) of the line. By this we partition the territory design problem for  $V'$  into two disjoint subproblems, one for  $V'_l$  and one for  $V'_r$ . These subproblems are then solved independently from one another again by dividing each of them along a line. This iterative partitioning into subproblems gives the heuristic its name: successive dichotomies (termed in Ricca and Simeone [RS97]).

Since a problem that is not trivial generates two subproblems, the problems our heuristic examines are related according to a binary tree. The root of the tree is the problem we start with and the leaves correspond to territories.

Figure 4 shows an example of partitioning the original problem with basic areas  $V$  into two disjoint subproblems with basic areas  $V_l$  and  $V_r$ , respectively. Figure 5 illustrates the two subproblems generated by the solution of a problem.

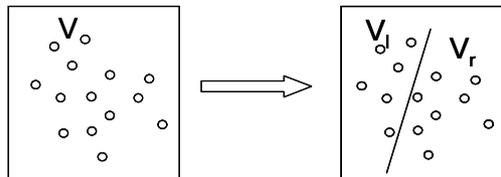


Figure 4: A partitioning of problem  $V$  into two disjoint subproblems with basic areas  $V_l$  and  $V_r$ , respectively.

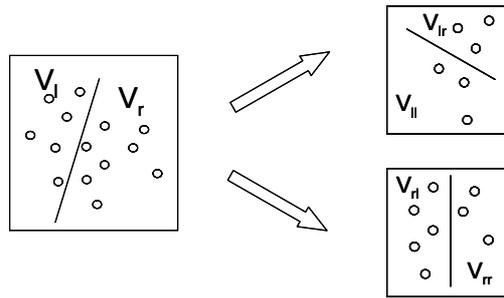


Figure 5: Every problem generates two subproblems.

Our heuristic explores the binary tree with nodes corresponding to problems and terminates when all leaves are generated. Two questions need to be answered:

- How do we perform the partitioning of a problem into subproblems? (Section 6.2)
- How do we explore the tree? (Section 6.3)

## 6.2 Solving the basic problem

The initial problem is to partition  $V$  into  $p$  territories. An instance of a (sub-)problem (called *basic problem*) is defined by  $V' \subseteq V$  and a positive number  $p' \leq p$ . A basic problem with  $p' = 1$  is trivial, since then  $V'$  defines a territory. If  $p' > 1$  we solve the problem by choosing a line and numbers  $p'_l, p'_r \geq 1$  with  $p'_l + p'_r = p'$ . This yields two new subproblems  $(V'_l, p'_l)$  and  $(V'_r, p'_r)$  that replace problem  $(V', p')$ .

The method to solve the basic problem is designed to take the criteria of balance and compactness into account. Further it is important that it runs fast, since many basic problems need to be solved in the search tree.

In an instance of the basic problem we are given a subset  $V'$  of basic areas as points in the plane and a number  $p' \geq 1$ . As already mentioned above we have to make two decisions:

1. Select  $p'_l, p'_r \geq 1$  with  $p'_l + p'_r = p'$ .
2. Select a line to partition  $V'$  into two subsets  $V'_l$  and  $V'_r$  of points left of and right of the line, respectively.

How  $p'_l$  and  $p'_r$  are selected depends on whether  $p'$  is even or odd. If  $p'$  is even we simply set  $p'_l = p'_r = p'/2$ . If  $p'$  is odd we consider two cases,

$$p'_l = \left\lceil \frac{p'}{2} \right\rceil, p'_r = \left\lfloor \frac{p'}{2} \right\rfloor \quad \text{and} \quad p'_l = \left\lfloor \frac{p'}{2} \right\rfloor, p'_r = \left\lceil \frac{p'}{2} \right\rceil.$$

For the second decision one could imagine to consider more general methods to define a partition of  $V'$  than separating the points along a line. But it has two advantages to do it in this way, stated in the following propositions.

**Proposition 1** *If the basic problem is solved by partitioning  $V'$  into two parts by a separating line, we yield territories which have (when considered as subsets of  $V$ ) pairwise disjoint convex hulls.*

**Proof:** Obviously  $V'_l$  and  $V'_r$  have disjoint convex hulls. Apply this argument recursively.  $\square$

In Proposition 1 we assume that none of the points in  $V'$  is located on the separating line. However the statement stays true if we assume that points located on the line are always included into  $V'_l$ .

**Proposition 2** *If no three points in  $V'$  lie on a common line, the number of partitions of  $V'$  along a line is bounded by  $|V'|^2$ .*

**Proof:** Each such partition is induced by an ordered pair  $(v, u)$  of (not necessarily distinct) points in  $V'$  in the following way: If  $v \neq u$  they define a unique ordered line, we define  $V'_l$  to contain all points left of the line together with  $v$  and  $u$ . If  $v = u$  and  $v$  can be separated from the other points in  $V'$  by a line we set  $V_l = \{v\}$ .  $\square$

## Generating partitions

Proposition 2 limits the number of partitions that are interesting to be considered by a quadratic term. Unfortunately this is too much for large scale problems. Therefore we decided to examine not all of these partitions. Instead only those partitions of  $V'$  are considered that are generated by lines with some fixed directions. Only a small number of directions is used. This seems to be rather restrictive but we found that it produces very good results. The major advantage however is that all partitions generated by lines of a fixed direction can be examined very fast.

To explain why, let the direction be given by  $\alpha \in [0, \pi)$ , the angle of the line with the positive x-axis. Let us first assume that  $\alpha = \pi/2$ , i.e. we consider separating lines parallel to the y-axis. Before examining the partitions generated by such lines, we sort the points in  $V'$  by non-decreasing x-coordinate  $x_v$ . It is clear that every possible partition along a line parallel to the y-axis divides this sorted sequence into a left and a right part. To examine all partitions we only have to examine all subdivisions of the sequence into a left and a right part. Thus there are as many (nontrivial) partitions as points in the sequence minus one, which is linear in  $|V'|$ .

See Figure 6 for an example. Every vertical line, i.e. a line parallel to the y-axis, through each of the points generates a partition of the original problem into two subproblems.

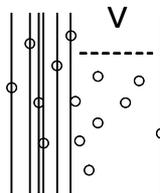


Figure 6: Possible partitions of the problem using vertical lines.

If  $\alpha$  is different from  $\pi/2$  the same idea applies after rotating the coordinate system so that the line through the origin with angle  $\alpha$  becomes the y-axis. Then again we sort the

points by non-decreasing x-coordinate. The new x-coordinates of the points after rotating the coordinate system are given as

$$x_v \sin \alpha + y_v \cos \alpha.$$

Before we explain how we examine a partition of  $V'$  under the criteria of balance and compactness, we summarize how the partitions that we consider are generated.

**Step 1.** Select a number  $N \geq 2$  of line directions to consider.

**Step 2.** For  $i = 0, 1, \dots, N - 1$  let  $\alpha_i = \pi/i$ .

**Step 3.** Consider direction  $\alpha_i$ : sort the points in  $V'$  by non-decreasing value of  $x_v \sin \alpha_i + y_v \cos \alpha_i$ . Let this sequence be denoted  $v_1, v_2, \dots, v_s$ .

**Step 4.** For  $k = 1, 2, \dots, s - 1$  "examine" the partition given by

$$V'_l = \{v_1, \dots, v_k\} \text{ and } V'_r = \{v_{k+1}, \dots, v_s\}.$$

We repeat steps 3 and 4 for all  $N$  directions. We found that  $N = 8$  or  $16$  provide good results.

### Examining a partition

The quality of a partition  $V'_l, V'_r$  of  $V'$  and  $p'_l + p'_r = p'$  depends mainly on two factors.

- What is the size of the average activity measures  $w(V'_l)/p'_l$  and  $w(V'_r)/p'_r$ ? (Balance)
- How 'compact' are (the convex hulls of)  $V'_l$  and  $V'_r$ ? (Compactness)

### Balance

First we discuss balance. Ideally we would have  $w(V'_l)/p'_l = w(V'_r)/p'_r = w(V')/p'$ , since then we would finally get territories with exactly the same size. Due to the discrete nature of the problem this is generally not possible.

Therefore we try to come as close as possible to perfect balance. In the sequence  $v_1, \dots, v_s$  of Step 3 above we determine an index  $k$  such that

$$w(\{v_1, \dots, v_{k-1}\}) < (p'_l/p') w(V') \text{ and } w(\{v_1, \dots, v_k\}) \geq (p'_l/p') w(V') \quad (12)$$

(If all  $w_v$  are positive  $k$  is unique.) Only the partition generated for this value  $k$  is considered further. All other partitions generated in step 4 above are not balanced enough. But also the partition for  $k$  will be discarded if it is *infeasible*. This is the case when  $k < p'_l$  or  $s - k < p'_r$  or when  $w(V'_l)/p'_l$  or  $w(V'_r)/p'_r$  is not in the interval  $[L, U]$ .

Consequently for each direction  $\alpha_i$  we consider between zero and two feasible partitions, depending also on whether  $p'$  is even or odd. All these partitions are then ranked according to the compactness criterion presented next.

### Compactness

Every partition we consider is generated by a line  $L$  which is defined by the direction  $\alpha_i$  and the location of basic area  $v_k$  according to (12). To find a compact territory design we use a measure that is based on the following reasoning. The segment of  $L$  that lies "within"  $V'$  will contribute to the total length of territory borders in the final territory layout. If we try to make this segment short we can hope to end up with a small total border length, and therefore with a compact layout.

For example in Figure 7 two possible choices of lines for partitioning a given set of basic areas into two smaller subproblems are illustrated. Intuitively the line on the right-hand side will yield more compact territories than the one on the left-hand side.

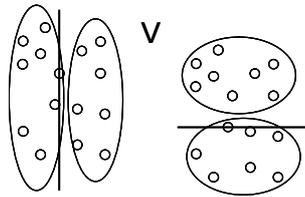


Figure 7: Two possible partitions with different compactness.

Since  $V'$  is a discrete set of points, it is not clear however what the length of the intersection of line  $L$  with  $V'$  is. We use two methods to define this length.

The first one is to use the length of the intersection of  $L$  with the convex hull  $C$  of  $V'$ . By convexity if  $v_k$  is inside of  $C$  we see that  $L$  intersects  $C$  in two points. The Euclidian distance of these two points defines the length of the segment (Figure 8, left picture). If  $v_k$  is a vertex of  $C$  the length can be zero. See Figure 8 left-hand side picture.

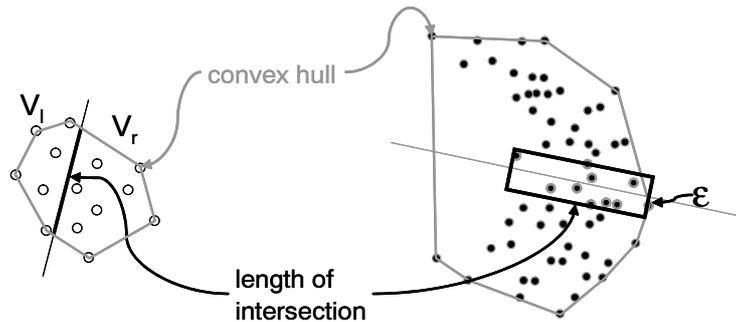


Figure 8: Two options to determine the length of the intersecting line: intersection with the convex hull or using a stripe.

Using the convex hull works well if the points in  $V'$  are uniformly distributed within  $C$ . Typically this is the case when  $|V'|$  is not very large. But consider the example of Figure 8, right-hand side. Here the convex hull does not describe the distribution of the points in  $V'$  well, and the length of the segment of  $L$  within the hull does not give the right information on how long the part  $L$  within  $V'$  is.

Therefore if  $|V'|$  is large we use a different method to measure compactness. We consider all points of  $V'$  that are close to  $L$ , i.e. lie in a stripe whose width is a fixed percentage of the width of the hull  $C$ . (Width measured orthogonally to  $L$ .) We project these points onto  $L$  and define the largest distance between any two of the projections as length of the segment of  $L$  that lies within  $V'$ .

### 6.3 Search tree to find a good territory design

In the last section we explained how a basic problem is "solved" by partitioning it into two subproblems. Since several line directions are considered we have different partitions into subproblems. In order to choose an appropriate partition for the subdivision all of them are ranked by heuristic measures for balance and compactness.

The straightforward "greedy" approach to realize just the best partition according to this ranking is however not sufficient. Even though only the best balanced partition among those possible for a certain line direction is considered there is no guarantee that one does not encounter an infeasible subproblem later, i.e. one with  $w(V')/p'$  outside the interval  $[L, U]$ .

Therefore we incorporated a backtracking mechanism into our heuristic. It allows to revisit a basic problem at a higher level to revise the division made there. We then perform the next partition according to our ranking and continue the search. In the following we explain the search mechanism more formally.

#### The search tree

A node  $\varphi = (V_\varphi, p_\varphi)$  of the search tree corresponds to a basic problem: subdivide  $V_\varphi$  into  $p_\varphi$  territories. The status of a node can be *active*, *inactive* or *isLeaf*. The latter is the case if  $p_\varphi$  equals one. The root node is  $\varphi_0 = (V, p)$ . It is active at the beginning of the search.

In each iteration of the search, an active node  $\varphi = (V_\varphi, p_\varphi)$  is selected. If  $p_\varphi = 1$  the status of the node is set to *isLeaf*. Otherwise it is set to *inactive*, and by using the highest ranked unused feasible partition for the basic problem of this node, two new active nodes  $\varphi_l = (V_{\varphi_l}, p_{\varphi_l})$  and  $\varphi_r = (V_{\varphi_r}, p_{\varphi_r})$  are generated. Here  $V_{\varphi_l}$  ( $V_{\varphi_r}$ ) are the basic areas left (right) of the dividing line. Now all feasible partitions for the two generated subproblems  $\varphi_l$  and  $\varphi_r$  are computed and ranked due to the balance and compactness criterion.

The search terminates when no active nodes are left. The set of leaf nodes then corresponds to a territory plan. If for an active node  $\varphi$  and its corresponding basic problem no feasible partitions are left, a backtrack operation is performed as follows. The father node of  $\varphi$ , which is inactive, is made active again and all its descendant nodes are deleted. Afterwards the search continues with this node.

If the situation occurs that we have to backtrack from the root node it is proved that the problem is infeasible. This occurs if  $L$  and  $U$  are defined too constraining (under the selected number of line directions).

#### Limiting the size of the search tree

The search encounters at least  $2p - 1$  active nodes until it terminates, this is the minimum number of nodes of a binary tree with  $p$  leaves. Due to backtracking operations however the

number of nodes examined can be much larger. Especially proving infeasibility of the problem requires to examine all feasible partitions for all basic problems, in general this number is exponential.

Therefore it is necessary to limit the search. One possibility is to stop after a maximum number of nodes has been explored and to output that no feasible (with respect to  $L$  and  $U$ ) territory design has been found.

We chose another way since it seemed better to us to output some result, even an infeasible one, instead of no result. Therefore, after a certain node limit is reached, we decrease  $L$  and increase  $U$  by some amount and thus enlarge the number of feasible partitions. We do not restart the search so the relaxed bounds apply only to newly generated nodes of the search tree. The change in  $L$  and  $U$  is made in such a way that the tolerance  $\tau$  (see (11)) is doubled. This relaxation mechanism is repeated a few times if necessary. If then the search still does not terminate, we finally set  $L$  to zero and  $U$  to infinity. Afterwards the search performs no more backtracking and terminates quickly.

#### 6.4 Outline of the successive dichotomies heuristic

Now a rough outline of the successive dichotomies heuristic will be given:

**Input** Set of basic areas  $V$  with corresponding activity measures  $w_v$ ,  $v \in V$ , and number of territories  $p$ . Parameter  $\tau$ .

##### Step 1 Initialization

Compute the values  $L = (1 - \tau) w(V)/p$  and  $U = (1 + \tau) w(V)/p$ .

Set the status of the root node  $\varphi_0 = (V, p)$  to *active* and compute and rank all feasible partitions.

##### Step 2 While there are *active* nodes left

Let  $\varphi = (V_\varphi, p_\varphi)$  be an *active* node.

*/\* Leaf node \*/*

**If**  $p_\varphi = 1$  **then** set the status of  $\varphi$  to *isLeaf*. **Continue** with *Step 2*.

*/\* Backtrack \*/*

**If** there are no more feasible partitions for  $\varphi$  left **then**

**If**  $\varphi = \varphi_0$  is the root node

**then** relax  $L$  and  $U$  and compute and rank again all feasible partitions of  $\varphi_0$ .

**Continue** with *Step 2*.

**else** set the father node  $\varphi_f$  of  $\varphi$  to *active* and delete all descendant nodes of  $\varphi_f$ .

**Continue** with *Step 2*.

*/\* Partition \*/*

Implement the highest ranked partition creating two new *active* nodes  $\varphi_l = (V_{\varphi_l}, p_{\varphi_l})$  and  $\varphi_r = (V_{\varphi_r}, p_{\varphi_r})$ . Delete this partition from the list of partitions of node  $\varphi$ . Compute and rank all feasible partitions of  $\varphi_l$  and  $\varphi_r$ .

Set  $\varphi$  to *inactive*.

```
/* Limiting search tree */
```

```
If some (node) limit is exceeded then relax  $L$  and  $U$ .
```

**Output** A territory design made up of all nodes with status *isLeaf*.

In Figure 9 an example of two sales territory alignments of German zip-code areas (indicated as points) into 70 territories created by applying the above heuristic is presented. Two different sets of line directions were used: one with 2 (left-hand side image) and the other with 16 directions (right-hand side picture).

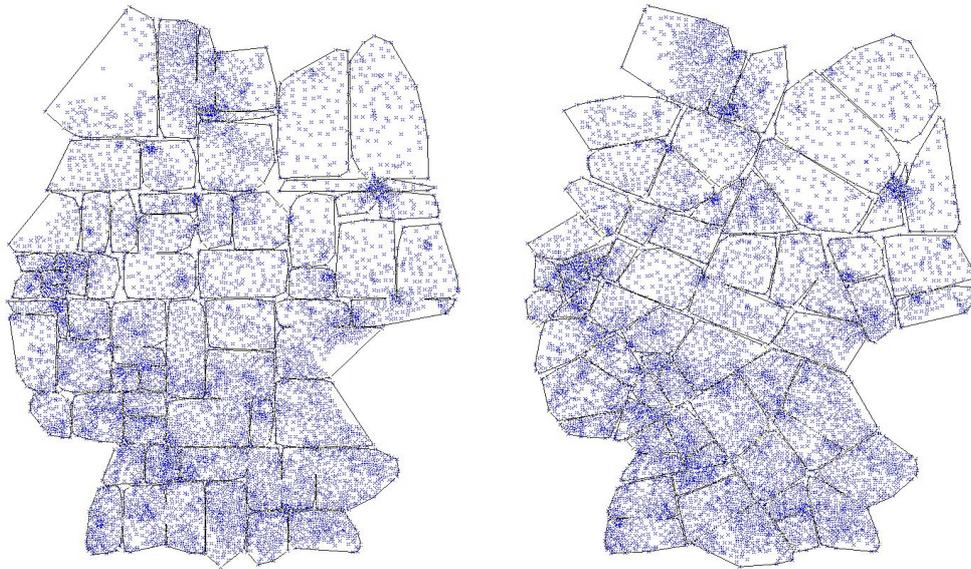


Figure 9: 70 territories based on German zip-code areas.

### 6.5 Combination of successive dichotomies with optimal split resolution

Here we want to sketch how the methods in Sections 5 and 6 can be combined to yield a modified successive dichotomies heuristic with a priori worst case bound on the deviation of the territory sizes from the average size.

The idea how to combine the methods is fairly simple, and relates to the way in which the basic problem is solved in 6.2. There we partition the subset  $V'$  into two subsets  $V'_l$  and  $V'_r$  of approximately equal size. Now, if in this process it is allowed to ‘split’ the elements in  $V'$ , it is clearly possible to achieve  $w(V'_l) = w(V'_r)$  by splitting at most one  $v \in V'$ .

Solving the basic problem with splitting allowed in this way during the search, we end up with territories of exactly the same size. Further if we consider these territories and the splitted basic areas as nodes of a graph, having edges between  $v \in V$  and  $B$  if a part of  $v$  belongs to  $B$ , we yield a split adjacency similar to the one in section 5.2.

The important observation here is that this split adjacency is again cycle-free. The reason is the recursive partitioning of  $V$  in the search. Therefore all the results of section 5.3 on optimal split resolution apply here also. Particularly the worst case bound  $\max\{w_v : v \in V^S\}$

for the maximum deviation of district sizes from average in terms of the maximum size of the splits holds.

Note that this modification of the successive dichotomies heuristic prevents also the necessity of backtracking. By combining successive dichotomies with optimal split resolution we yield a procedure for solving the territory design problem that is very fast and for which the balance of the resulting territories can be estimated in advance.

## 7 Computational results

In the following, we will present results indicating the computational efficiency of the successive dichotomies heuristic. They give a good idea of the performance of the method, both in running times and solution quality, and indicate its suitability for the use in an interactive environment. Actually, the results presented here are just an extract of our tests. They are representative for the typical behavior of the algorithms and the conclusions that we draw are in fact based on many computational tests of the algorithms.

In the following, we will compare the successive dichotomies heuristic, named *Dicho*, with two location–allocation based methods. The first one, called *Inter*, employs the AllocMinDist method in the allocation phase and a local search technique based on Teitz and Bart’s interchange method ([TB68]) in the location part. The second heuristic, called *Split*, uses TRANSP in the allocation phase and resolves split areas using the AssignMAX method. The location phase utilizes a Lagrangean relaxation method.

The three heuristics were tested on problems of different sizes in terms of the numbers of basic areas, starting with 100 up to 1000. For each number of basic areas several problem instances were generated. Each instance was solved with varying numbers of territories and different activity measures. The instances were created using real–world data obtained from the GIS *ArcView*. Basic areas correspond to German zip–code areas and the activity measures are different demographic figures. Every test problem was solved with each of the three heuristics *Inter*, *Split* and *Dicho* and the running time of the respective method and the quality of the resulting territories in terms of maximal relative percentage deviation of a territory from the average were obtained. For each heuristic these two values were then averaged over all problem instances with the same number of basic areas. The results are depicted in Figures 10 and 11.

Comparing the two location–allocation methods one can easily see that the better solution quality in terms of maximal deviation of the *Split* heuristic is traded off against a considerably larger solution time compared to the *Inter* heuristic. Moreover the *Dicho* algorithm outperforms in average the other two heuristics with respect to running time and solution quality for almost all problem sizes. This underlines the quality and speed of the successive dichotomies heuristic and stresses its suitability for the use in an interactive environment.

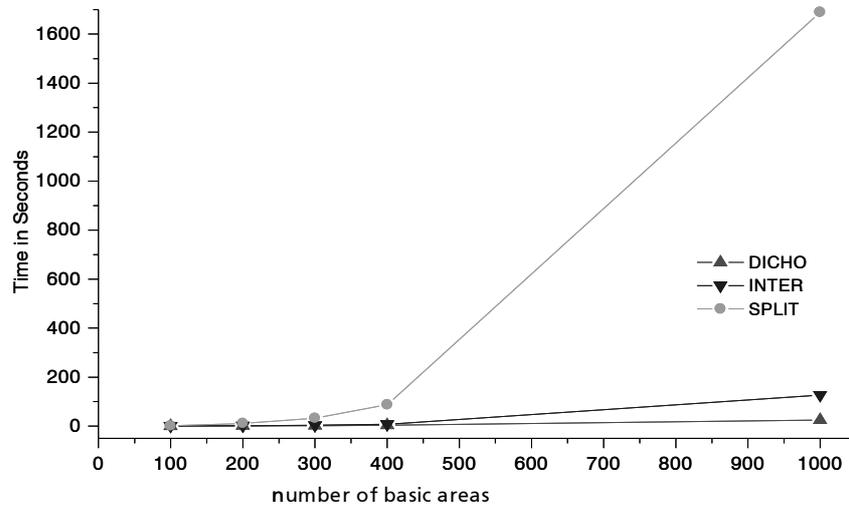


Figure 10: Computational results for a varying number of basic areas in terms of running times

## 8 Extensions and GIS-Integration

The heuristics presented in Sections 5 and 6 can be extended to take additional planning criteria or problem characteristics into account. For example

**Several activity measures** The heuristics can be extended to handle several activity measures. In this case while examining a partition (see section 6.2) one has to take all activity measures into account when determining the best balanced partition(s).

**Prescribed and forbidden territory centers** Another extension is the consideration of prescribed and forbidden territory centers. That means we are already given some fixed territory centers at the beginning which have to be taken into account or, the other way around, some basic areas are not allowed to be selected as district centers.

**Prescribed territories** In case some districts are already given at the beginning of the planning process the methods can be adapted to take the already existing territories into account and possibly add additional basic areas to them.

**Connectedness** Finally, if neighborhood information about the basic areas is given, i.e. we know if two basic areas are neighboring or not, then the heuristics can be extended in such a way that they always yield connected territories (if possible).

Although the above mentioned extensions can be applied to location-allocation heuristics as well as to the successive dichotomies method one has to note that the latter heuristic is far more flexible in terms of incorporating extensions which do not rely on linear relationships, for example complex measures for compactness.

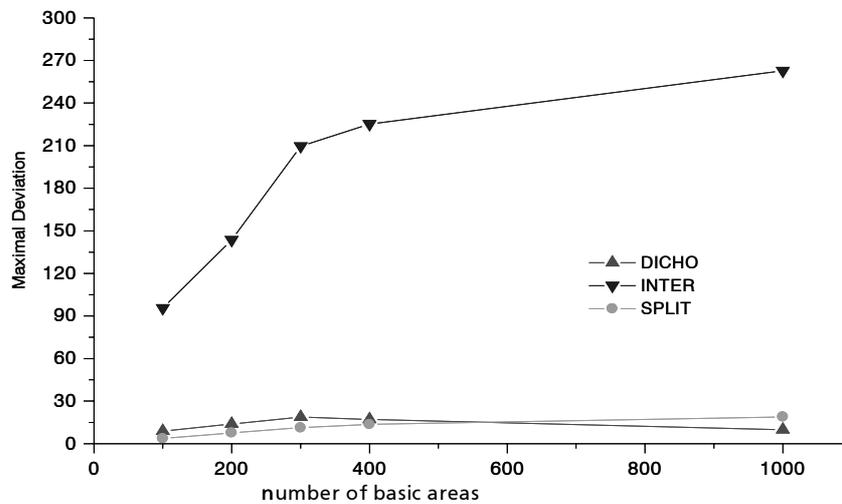


Figure 11: Computational results for a varying number of basic areas in terms of solution quality.

Moreover the heuristics can be incorporated into a larger framework in order to apply them to different practical planning problems, as outlined in the introduction. For example scenarios where not all basic areas have to be (or can be) partitioned into territories due to budget constraints. Or applications where a limit on the maximal allowed geographic extend of the territories has to be taken into account.

In addition, the number  $p$  of territories need not be fixed in advance. Instead, the algorithm will choose the appropriate number of districts in such a way that the planning criteria are best fulfilled. For example, partition the basic areas in the region under consideration into as few as possible territories such that the size of all territories is below a certain maximal bound.

### Integration into GIS

Enhanced with these extensions the successive dichotomies heuristic is the algorithmic base of a commercial software product for geo-marketing called *BusinessManager*. The BusinessManager is an extension of ESRI's ArcView GIS and has been developed by *geomer GmbH* together with *Fraunhofer ITWM*.

In the BusinessManager the user can solve general territory design problems. The interaction is integrated with the GIS so the user can access data from arbitrary shape files. The basic areas can be defined by points, lines, polygons etc, depending of the planning problem under consideration.

Figure 12 shows a screenshot of the BusinessManager software.

The user benefits from this integration of optimization algorithms into a GIS in several ways. Firstly, GIS are a common tool in geo-marketing and the user has access to all GIS functionality to work on his planning problem. Secondly the seamless integration of territory

planning heuristics allows the user to access these methods without being an expert in Operations Research. After the computations performed by the heuristics in the background are finished an immediate visualization of the results in the GIS allows the user to examine the proposed solution. Then he has the option to manually adjust the solution or to change the planning parameters and start a new run of the optimization engine. It is this interactive type of work with the heuristics that requires the fast generation of solutions, often mentioned in this paper.

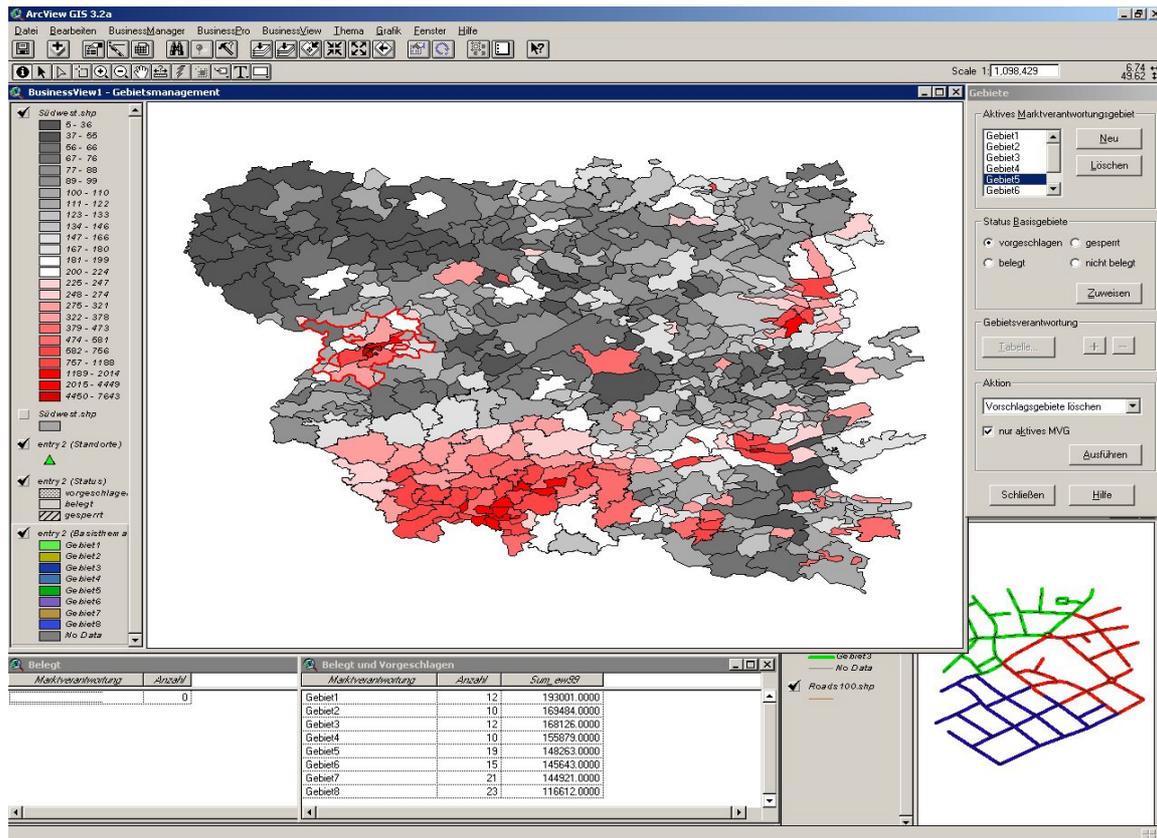


Figure 12: Screenshot of the BusinessManager software.

The technical side of the integration into the GIS is sketched in Figure 13. While the user interaction and data management is all done within the GIS there is the optimization engine as an underlying part. We found it useful to distinguish two layers in the optimization engine. The lower layer contains the implementation of the heuristics. Since generally the planning problem specified by the user in the GIS can not be mapped in a direct way to one of the heuristics (or there had to be a quite large number of them), an intermediate layer contains the so-called *scenario manager*. This layer selects and combines the algorithms in the heuristics layer that are suited to produce an answer to the user's planning problem. As an example the scenario layer calls the successive dichotomies heuristic repeatedly with varying  $p$  if the number of territories is asked as part of the planning result by the user.

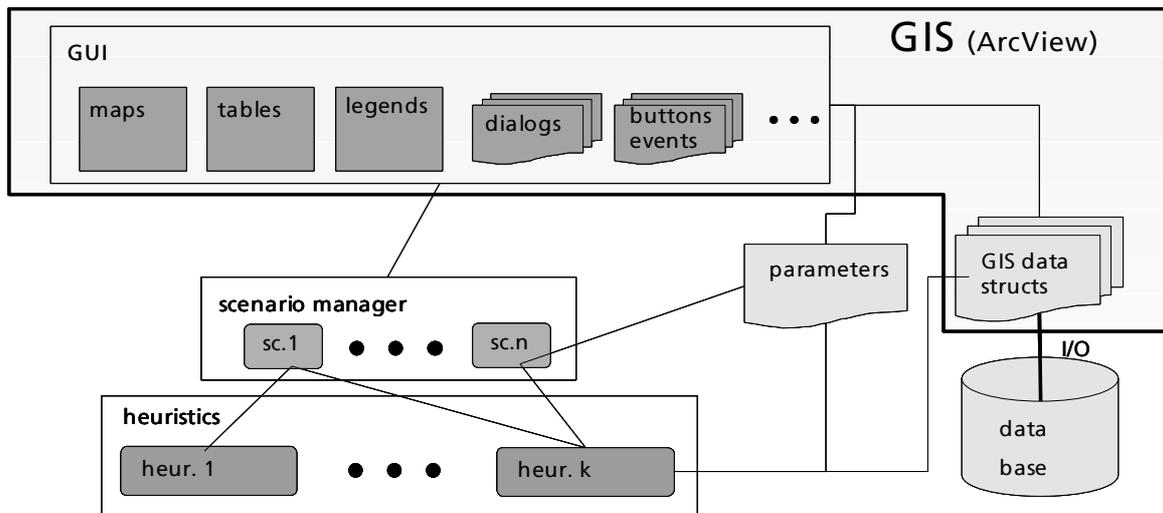


Figure 13: Integration of the heuristics into ArcView GIS.

## 9 Conclusions

Problems of territory alignment arise in different application areas. Our main purpose in this paper was to show how the planner can be adequately supported to solve such problems in practice and the role of operations research in this process.

From the many proposed algorithmic ideas how to solve territory design problems, two heuristic approaches are discussed more in-depth in this paper. The first one is based on the location–allocation principle. In the allocation phase we contribute a method to solve the split resolution problem in an optimal fashion. However, even if the instances of the transportation problem in the allocation phase can be solved efficiently, we found that on large-scale problems the running times were still too high.

Therefore we detail out a heuristic approach, so far only sketched in the literature, that solves the territory design problem geometrically. This successive dichotomies heuristic proves to be very fast and flexible. All the necessary requirements for the heuristic are basic procedures in computational geometry: polygon–line intersection, convex hull, coordinate transformation (rotation) etc. These are computationally fast and easy to implement. Especially in contrast to most of the classical methods there is no need for specialized solvers or methods for mathematical programming problems like for the transportation problem. Despite its simplicity the successive dichotomies heuristic provides surprisingly good results.

We further described how the heuristics for territory design have been integrated into a commercial software for geo-marketing. This allows planners to use these heuristics for various planning problems in territory design without being operations research experts.

On the other hand, as indicated in Section 8, there is still a lot of work to do for operations researchers in the area of territory design, both on the theoretical and the practical side.

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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 rarefied gas flows Part I: Coverage locally at equilibrium**

A new approach is proposed to model and simulate numerically heterogeneous catalysis in rarefied gas flows. It is developed to satisfy all together the following points:

- 1) describe the gas phase at the microscopic scale, as required in rarefied flows,
- 2) describe the wall at the macroscopic scale, to avoid prohibitive computational costs and consider not only crystalline but also amorphous surfaces,
- 3) reproduce on average macroscopic laws correlated with experimental results and
- 4) derive analytic models in a systematic and exact way. The problem is stated in the general framework of a non static flow in the vicinity of a catalytic and non porous surface (without aging). It is shown that the exact and systematic resolution method based on the Laplace transform, introduced previously by the author to model collisions in the gas phase, can be extended to the present problem. The proposed approach is applied to the modelling of the EleyRideal and LangmuirHinshelwood recombinations, assuming that the coverage is locally at equilibrium. The models are developed considering one atomic species and

extended to the general case of several atomic species. Numerical calculations show that the models derived in this way reproduce with accuracy behaviors observed experimentally.

(24 pages, 1998)

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

## **Efficient Texture Analysis of Binary Images**

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

(17 pages, 1998)

9. J. Orlik

## **Homogenization for viscoelasticity of the integral type with aging and shrinkage**

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

(20 pages, 1998)

10. J. Mohring

## **Helmholtz Resonators with Large Aperture**

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

(21 pages, 1998)

11. H. W. Hamacher, A. Schöbel

### **On Center Cycles in Grid Graphs**

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

12. H. W. Hamacher, K.-H. Küfer

### **Inverse radiation therapy planning - a multiple objective optimisation approach**

For some decades radiation therapy has been proved successful in cancer treatment. It is the major task of clinical radiation treatment planning to realize on the one hand a high level dose of radiation in the cancer tissue in order to obtain maximum tumor control. On the other hand it is obvious that it is absolutely necessary to keep in the tissue outside the tumor, particularly in organs at risk, the unavoidable radiation as low as possible.

No doubt, these two objectives of treatment planning - high level dose in the tumor, low radiation outside the tumor - have a basically contradictory nature. Therefore, it is no surprise that inverse mathematical models with dose distribution bounds tend to be infeasible in most cases. Thus, there is need for approximations compromising between overdosing the organs at risk and underdosing the target volume.

Differing from the currently used time consuming iterative approach, which measures deviation from an ideal (non-achievable) treatment plan using recursively trial-and-error weights for the organs of interest, we go a new way trying to avoid a priori weight choices and consider the treatment planning problem as a multiple objective linear programming problem: with each organ of interest, target tissue as well as organs at risk, we associate an objective function measuring the maximal deviation from the prescribed doses.

We build up a data base of relatively few efficient solutions representing and approximating the variety of Pareto solutions of the multiple objective linear programming problem. This data base can be easily scanned by physicians looking for an adequate treatment plan with the aid of an appropriate online tool. (14 pages, 1999)

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

### **On the Analysis of Spatial Binary Images**

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

14. M. Junk

### **On the Construction of Discrete Equilibrium Distributions for Kinetic Schemes**

A general approach to the construction of discrete equilibrium distributions is presented. Such distribution functions can be used to set up Kinetic Schemes as well as Lattice Boltzmann methods. The general prin-

ciples 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 Wickseil's Corpuscle Problem**

Wickseil'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, Wickseil's problem is an inverse problem where the interesting size distribution is the unknown part of a Volterra equation. The problem is often regarded ill-posed, because the structure of the integrand implies unstable numerical solutions. The accuracy of the numerical solutions is considered here using the condition number, which allows to compare different numerical methods with different (equidistant) class sizes and which indicates, as one result, that a finite section thickness of the probe reduces the numerical problems. Furthermore, the relative error of estimation is computed which can be split into two parts. One part consists of the relative discretization error that increases for increasing class size, and the second part is related to the relative statistical error which increases with decreasing class size. For both parts, upper bounds can be given and the sum of them indicates an optimal class width depending on some specific constants. (18 pages, 1999)

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

### **Solving nonconvex planar location problems by finite dominating sets**

It is well-known that some of the classical location problems with polyhedral gauges can be solved in polynomial time by finding a finite dominating set, i.e. a finite set of candidates guaranteed to contain at least one optimal location.

In this paper it is first established that this result holds for a much larger class of problems than currently considered in the literature. The model for which this result can be proven includes, for instance, location problems with attraction and repulsion, and location-allocation problems.

Next, it is shown that the approximation of general gauges by polyhedral ones in the objective function of our general model can be analyzed with regard to the subsequent error in the optimal objective value. For the approximation problem two different approaches are described, the sandwich procedure and the greedy

algorithm. Both of these approaches lead - for fixed epsilon - to polynomial approximation algorithms with accuracy epsilon for solving the general model considered in this paper.

*Keywords: Continuous Location, Polyhedral Gauges, Finite Dominating Sets, Approximation, Sandwich Algorithm, Greedy Algorithm* (19 pages, 2000)

19. A. Becker

### **A Review on Image Distortion Measures**

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

*Keywords: Distortion measure, human visual system* (26 pages, 2000)

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

### **Polyhedral Properties of the Uncapacitated Multiple Allocation Hub Location Problem**

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

*Keywords: integer programming, hub location, facility location, valid inequalities, facets, branch and cut* (21 pages, 2000)

21. H. W. Hamacher, A. Schöbel

### **Design of Zone Tariff Systems in Public Transportation**

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

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

### **The Finite-Volume-Particle Method for Conservation Laws**

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

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

### **Location Software and Interface with GIS and Supply Chain Management**

The objective of this paper is to bridge the gap between location theory and practice. To meet this objective focus is given to the development of software capable of addressing the different needs of a wide group of users. There is a very active community on location theory encompassing many research fields such as operations research, computer science, mathematics, engineering, geography, economics and marketing. As a result, people working on facility location problems have a very diverse background and also different needs regarding the software to solve these problems. For those interested in non-commercial applications (e. g. students and researchers), the library of location algorithms (LoLA can be of considerable assistance. LoLA contains a collection of efficient algorithms for solving planar, network and discrete facility location problems. In this paper, a detailed description of the functionality of LoLA is presented. In the fields of geography and marketing, for instance, solving facility location problems requires using large amounts of demographic data. Hence, members of these groups (e. g. urban planners and sales managers) often work with geographical information too. 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, Walldorf, Germany. The paper ends with some conclusions and an outlook to future activities.

*Keywords: facility location, software development, geographical information systems, supply chain management*  
(48 pages, 2001)

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

### **Mathematical Modelling of Evacuation Problems: A State of Art**

This paper details models and algorithms which can be applied to evacuation problems. While it concentrates on building evacuation many of the results are applicable also to regional evacuation. All models consider the time as main parameter, where the travel time between components of the building is part of the input and the overall evacuation time is the output. The paper distinguishes between macroscopic and microscopic evacuation models both of which are able to capture the evacuees' movement over time. Macroscopic models are mainly used to produce good lower bounds for the evacuation time and do not consider any individual behavior during the emergency situation. These bounds can be used to analyze existing buildings or help in the design phase of planning a building. Macroscopic approaches which are based on dynamic network flow models (minimum cost dynamic flow, maximum dynamic flow, universal maximum flow, quickest path and quickest flow) are described. A special feature of the presented approach is the fact, that travel times of evacuees are not restricted to be constant, but may be density dependent. Using 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 Akademierpreises 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 satisfied exactly by the coefficients in the Chapman-Enskog expansion. The distribution functions are naturally expressed in the local interfacial coordinates. The macroscopic quantities at the interface are extracted from the least-square solutions of a locally linearized system obtained from the known distribution functions. The proposed method does not require any geometric front construction and is robust for any interfacial topology. Simulation results of realistic filling process are presented: rectangular cavity in two dimensions and Hammer box, Campbell box, Sheffield box, and Motorblock in three dimensions. To enhance the stability at high Reynolds numbers, various upwind-type schemes are developed. Free-slip and no-slip boundary conditions are also discussed.

*Keywords: Lattice Boltzmann models; free-surface phenomena; interface boundary conditions; filling processes; injection molding; volume of fluid method; interface boundary conditions; advection-schemes; upwind-schemes*  
(54 pages, 2002)

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

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

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

*Keywords: traffic flow, macroscopic equations, kinetic derivation, multivalued fundamental diagram, stop and go waves, phase transitions*  
(25 pages, 2002)

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

### **Parameter influence on the zeros of network determinants**

To a network  $N(q)$  with determinant  $D(s;q)$  depending on a parameter vector  $q \in \mathbb{R}^r$  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-Khintchine theorem for the power spectrum are used to two ends: First, well known second order characteristics like the covariance can be estimated faster than usual via frequency space. Second, the Bartlett spectrum and the power spectrum can be used as second order characteristics in frequency space. Examples show, that in some cases information about the random closed set is easier to obtain from these characteristics in frequency space than from their real world counterparts.

*Keywords: Random set, Bartlett spectrum, fast Fourier transform, power spectrum*  
(28 pages, 2002)

38. D. d'Humières, I. Ginzburg

### **Multi-reflection boundary conditions for lattice Boltzmann models**

We present a unified approach of several boundary conditions for lattice Boltzmann models. Its general framework is a generalization of previously introduced schemes such as the bounce-back rule, linear or quadratic interpolations, etc. The objectives are two fold: first to give theoretical tools to study the existing boundary conditions and their corresponding accuracy; secondly to design formally third-order accurate boundary conditions for general flows. Using these boundary conditions, Couette and Poiseuille flows are exact solution of the lattice Boltzmann models for a Reynolds number  $Re = 0$  (Stokes limit).

Numerical comparisons are given for Stokes flows in periodic arrays of spheres and cylinders, linear periodic array of cylinders between moving plates and for Navier-Stokes flows in periodic arrays of cylinders for  $Re < 200$ . These results show a significant improvement of the overall accuracy when using the linear interpolations instead of the bounce-back reflection (up to an order of magnitude on the hydrodynamics fields). Further improvement is achieved with the new multi-reflection boundary conditions, reaching a

level of accuracy close to the quasi-analytical reference solutions, even for rather modest grid resolutions and few points in the narrowest channels. More important, the pressure and velocity fields in the vicinity of the obstacles are much smoother with multi-reflection than with the other boundary conditions.

Finally the good stability of these schemes is highlighted by some simulations of moving obstacles: a cylinder between flat walls and a sphere in a cylinder.

*Keywords: lattice Boltzmann equation, 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 cannot satisfactorily map the different backgrounds of physicians and the patient dependent necessities. So, too often a time consuming iteration process between evaluation of dose distribution and redefinition of the evaluation function is needed.

In this paper we propose a generic multi-criteria approach based on Pareto's solution concept. For each entity of interest - target volume or organ at risk a structure dependent evaluation function is defined measuring deviations from ideal doses that are calculated from statistical functions. A reasonable bunch of clinically meaningful Pareto optimal solutions are stored in a data base, which can be interactively searched by physicians. The system guarantees dynamical planning as well as the discussion of tradeoffs between different entities.

Mathematically, we model the upcoming inverse problem as a multi-criteria linear programming problem. Because of the large scale nature of the problem it is not possible to solve the problem in a 3D-setting without adaptive reduction by appropriate approximation schemes.

Our approach is twofold: First, the discretization of the continuous problem is based on an adaptive hierarchical clustering process which is used for a local refinement of constraints during the optimization procedure. Second, the set of Pareto optimal solutions is approximated by an adaptive grid of representatives that are found by a hybrid process of calculating extreme compromises and interpolation methods.

*Keywords: multiple criteria optimization, representative systems of Pareto solutions, adaptive triangulation, clustering and disaggregation techniques, visualization of Pareto solutions, medical physics, external beam radiotherapy planning, intensity modulated radiotherapy*  
(31 pages, 2003)

44. T. Halfmann, T. Wichmann

### **Overview of Symbolic Methods in Industrial Analog Circuit Design**

Industrial analog circuits are usually designed using numerical simulation tools. To obtain a deeper circuit understanding, symbolic analysis techniques can additionally be applied. Approximation methods which reduce the complexity of symbolic expressions are needed in order to handle industrial-sized problems. This paper will give an overview to the field of symbolic analog circuit analysis. Starting with a motivation, the state-of-the-art simplification algorithms for linear as well as for nonlinear circuits are presented. The basic ideas behind the different techniques are described, whereas the technical details can be found in the cited references. Finally, the application of linear and nonlinear symbolic analysis will be shown on two example circuits.

*Keywords: CAD, automated analog circuit design, symbolic analysis, computer algebra, behavioral modeling, system simulation, circuit sizing, macro modeling, differential-algebraic equations, index*  
(17 pages, 2003)

45. S. E. Mikhailov, J. Orlik

### **Asymptotic Homogenisation in Strength and Fatigue Durability Analysis of Composites**

Asymptotic homogenisation technique and two-scale convergence is used for analysis of macro-strength and fatigue durability of composites with a periodic structure under cyclic loading. The linear damage accumulation rule is employed in the phenomenologi-

cal 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 & Mladenović [HM97] for the p-median problem is described. An extensive numerical study is presented to show the efficiency of both heuristics and compare them.

*Keywords: genetic algorithms, variable neighborhood search, discrete facility location*  
(31 pages, 2003)

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

### **Exact Procedures for Solving the Discrete Ordered Median Problem**

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

*Keywords: discrete location, Integer programming*  
(41 pages, 2003)

48. S. Feldmann, P. Lang

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

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

*Keywords: Discrete linear systems, model reduction, stability, Hankel matrix, Stein equation*  
(16 pages, 2003)

49. J. Kallrath, S. Nickel

### **A Polynomial Case of the Batch Presorting Problem**

This paper presents new theoretical results for a special case of the batch presorting problem (BPSP). We will show 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 subdomain. A special implementation approach is used, which allows to perform unstructured local refinement in conjunction with the finite volume discretization. The multigrid - adaptive local refinement algorithm is tested on 2D Poisson equation and further is applied to a lid-driven flows in a cavity (2D and 3D case), comparing the results with bench-mark data. The software design principles of the solver are also discussed.

*Keywords: Navier-Stokes equations, incompressible flow, projection-type splitting, SIMPLE, multigrid methods, adaptive local refinement, lid-driven flow in a cavity* (37 pages, 2003)

55. V. Starikovicius

### **The multiphase flow and heat transfer in porous media**

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

*Keywords: Two-phase flow in porous media, variational formulations, global pressure, multiphase mixture model, numerical simulation* (30 pages, 2003)

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

### **Blocked neural networks for knowledge extraction in the software development process**

One of the main goals of an organization developing software is to increase the quality of the software while at the same time to decrease the costs and the duration of the development process. To achieve this, various decisions 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)

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

### **Largescale models for dynamic multi-commodity capacitated facility location**

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

*Keywords: supply chain management, strategic planning, dynamic location, modeling* (40 pages, 2003)

59. J. Orlik

### **Homogenization for contact problems with periodically rough surfaces**

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

*Keywords: asymptotic homogenization, contact problems* (28 pages, 2004)

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

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

In intensity-modulated radiotherapy (IMRT) planning the oncologist faces the challenging task of finding a treatment plan that he considers to be an ideal compromise of the inherently contradictory goals of delivering a sufficiently high dose to the target while widely sparing critical structures. The search for this a priori unknown compromise typically requires the computation of several plans, i.e. the solution of several optimization problems. This accumulates to a high computational expense due to the large scale of these problems – a consequence of the discrete problem formulation. This paper presents the adaptive clustering method as a new algorithmic concept to overcome these difficulties.

The computations are performed on an individually adapted structure of voxel clusters rather than on the original voxels leading to a decisively reduced computational complexity as numerical examples on real clinical data demonstrate. In contrast to many other similar concepts, the typical trade-off between a reduction in computational complexity and a loss in exactness can be avoided: the adaptive clustering method produces the optimum of the original problem. This flexible method can be applied to both single- and multi-criteria optimization methods based on most of the convex evaluation functions used in practice.

*Keywords: Intensity-modulated radiation therapy (IMRT), inverse treatment planning, adaptive volume structures, hierarchical clustering, local refinement, adaptive clustering, convex programming, mesh generation, multi-grid methods* (24 pages, 2004)

61. D. Kehrwald

### **Parallel lattice Boltzmann simulation of complex flows**

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

*Keywords: Lattice Boltzmann methods, parallel computing, microstructure simulation, virtual material design, pseudo-plastic fluids, liquid composite moulding* (12 pages, 2004)

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

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

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

*Keywords: Performance of iterative solvers, Preconditioners, Non-Newtonian flow* (17 pages, 2004)

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

### **On Modelling and Simulation of Different Regimes for Liquid Polymer Moulding**

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

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

64. T. Hanne, H. Neu

### **Simulating Human Resources in Software Development Processes**

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

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

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

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

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

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

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

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

### **Diffraction by image processing and its application in materials science**

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

68. H. Neunzert

### **Mathematics as a Technology: Challenges for the next 10 Years**

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

69. R. Ewing, O. Iliev, R. Lazarov, A. Naumovich

### **On convergence of certain finite difference discretizations for 1D poroelasticity interface problems**

Finite difference discretizations of 1D poroelasticity equations with discontinuous coefficients are analyzed. A recently suggested FD discretization of poroelasticity equations with constant coefficients on staggered grid, [5], is used as a basis. A careful treatment of the interfaces leads to harmonic averaging of the discontinuous coefficients. Here, convergence for the pressure and for the displacement is proven in certain norms for the scheme with harmonic averaging (HA). Order of convergence 1.5 is proven for arbitrary located interface, and second order convergence is proven for the case when the interface coincides with a grid node. Furthermore, following the ideas from [3], modified HA discretization are suggested for particular cases. The velocity and the stress are approximated with second order on the interface in this case. It is shown that for wide class of problems, the modified discretization provides better accuracy. Second order convergence for modified scheme is proven for the case when the interface coincides with a displacement grid node. Numerical experiments are presented in order to illustrate our considerations.  
*Keywords: poroelasticity, multilayered material, finite volume discretizations, MAC type grid, error estimates*  
(26 pages, 2004)

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

### **On Efficient Simulation of Non-Newtonian Flow in Saturated Porous Media with a Multigrid Adaptive Refinement Solver**

Flow of non-Newtonian in saturated porous media can be described by the continuity equation and the generalized Darcy law. Efficient solution of the resulting second order nonlinear elliptic equation is discussed here. The equation is discretized by a finite volume method on a cell-centered grid. Local adaptive refinement of the grid is introduced in order to reduce the number of unknowns. A special implementation approach is used, which allows us to perform unstructured local refinement in conjunction with the finite volume discretization. Two residual based error indicators are exploited in the adaptive refinement criterion. Second order accurate discretization on the interfaces between refined and non-refined subdomains, as well as on the boundaries with Dirichlet boundary condition, are presented here, as an essential part of the accurate and efficient algorithm. A nonlinear full approximation storage multigrid algorithm is developed especially for the above described composite (coarse plus locally refined) grid approach. In particular, second order approximation around interfaces is a result of a quadratic approximation of slave nodes in the multigrid - adaptive refinement (MG-AR) algorithm. Results from numerical solution of various academic and practice-induced problems are presented and the performance of the solver is discussed.  
*Keywords: Nonlinear multigrid, adaptive refinement, non-Newtonian in porous media*  
(25 pages, 2004)

71. J. Kalcsics, S. Nickel, M. Schröder

### **Towards a Unified Territory Design Approach – Applications, Algorithms and GIS Integration**

Territory design may be viewed as the problem of grouping small geographic areas into larger geographic clusters called territories in such a way that the latter are acceptable according to relevant planning criteria. In this paper we review the existing literature for applications of territory design problems and solution approaches for solving these types of problems. After identifying features common to all applications we introduce a basic territory design model and present in detail two approaches for solving this model: a classical location-allocation approach combined with optimal split resolution techniques and a newly developed computational geometry based method. We present computational results indicating the efficiency and suitability of the latter method for solving large-scale practical problems in an interactive environment. Furthermore, we discuss extensions to the basic model and its integration into Geographic Information Systems.  
*Keywords: territory design, political districting, sales territory alignment, optimization algorithms, Geographical Information Systems*  
(40 pages, 2005)

72. K. Schladitz, S. Peters, D. Reinel-Bitzer, A. Wiegmann, J. Ohser

### **Design of acoustic trim based on geometric modeling and flow simulation for non-woven**

In order to optimize the acoustic properties of a stacked fiber non-woven, the microstructure of the non-woven is modeled by a macroscopically homogeneous random system of straight cylinders (tubes). That is, the fibers are modeled by a spatially stationary random system of lines (Poisson line process), dilated by a sphere. Pressing the non-woven causes anisotropy. In our model, this anisotropy is described by a one parameter distribution of the direction of the fibers. In the present application, the anisotropy parameter has to be estimated from 2d reflected light microscopic images of microsections of the non-woven. After fitting the model, the flow is computed in digitized realizations of the stochastic geometric model using the lattice Boltzmann method. Based on the flow resistivity, the formulas of Delany and Bazley predict the frequency-dependent acoustic absorption of the non-woven in the impedance tube.

Using the geometric model, the description of a non-woven with improved acoustic absorption properties is obtained in the following way: First, the fiber thicknesses, porosity and anisotropy of the fiber system are modified. Then the flow and acoustics simulations are performed in the new sample. These two steps are repeated for various sets of parameters. Finally, the set of parameters for the geometric model leading to the best acoustic absorption is chosen.

*Keywords: random system of fibers, Poisson line process, flow resistivity, acoustic absorption, Lattice-Boltzmann method, non-woven*  
(21 pages, 2005)

Status quo: February 2005