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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

Fraunhofer Institut
Techno- und
Wirtschaftsmathematik

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

submitted to the proceedings of ECMI 2002

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Abstract

The *Folgar–Tucker equation* is used in flow simulations of fiber suspensions to predict fiber orientation depending on the local flow. In this paper[1] the essential parts of a complete, frame–invariant description of the *phase space* of this differential equation are presented for the first time.

keywords: fiber orientation, Folgar–Tucker equation, injection molding

[1] This paper is a slighlty extended version of the author's arcticle submitted for publication in the proceedings of the *ECMI 2002* conference. Due to space restrictions imposed by the editors, a large amount of the results presented in the author's talk at the conference as well as further details and (almost) all proofs had to be omitted. This material can be found in a forthcoming preprint [5] accompanying the present paper.

1 Introduction

The prediction of *fiber orientation* (FO) is an important component in a simulation of the injection molding process for short–fiber reinforced thermoplasts. The *Folgar–Tucker equation* (FTE)

$$\frac{D}{Dt}\hat{\mathbf{a}}^{(\mathbf{2})} \;=\; \hat{\mathbf{a}}^{(\mathbf{2})}\cdot\widehat{\mathbf{M}} + \widehat{\mathbf{M}}^{T}\cdot\hat{\mathbf{a}}^{(\mathbf{2})} - \left(\widehat{\mathbf{M}} + \widehat{\mathbf{M}}^{T}\right) : \hat{\mathbf{a}}^{(\mathbf{4})} + 2D_r\left[\hat{\mathbb{I}} - 3\hat{\mathbf{a}}^{(\mathbf{2})}\right] \qquad (1)$$

is the most frequently used model for FO calculation (see [1, 2] for further references and information on this subject). The dependent variable $\hat{\mathbf{a}}^{(\mathbf{2})}$ in (1), the so called *2nd order FO tensor* (or *FO matrix*), is a real symmetric 3×3 matrix defined as the 2nd moment of the FO distribution function. By construction the *eigenvalues* μ_k of $\hat{\mathbf{a}}^{(\mathbf{2})}$ are *nonnegative* and their sum (i.e. the *trace* of $\hat{\mathbf{a}}^{(\mathbf{2})}$) equals 1. This allows for an interpretation of an eigenvalue μ_k as the local fraction of fibers oriented along the direction of the corresponding eigenvector $\mathbf{E}_k$. In this sense the *spectral data* of the FO matrix represent the local macroscopic orientation state of the fibers within a small volume of the suspending fluid.

While the convective derivative on the l.h.s. of (1) describes the pure *transport* of the fibers in the local velocity field $\mathbf{U}(\mathbf{r},t)$ of the flow, the r.h.s. of (1) models the *rotational dynamics* of the fibers driven by the local velocity gradient $\widehat{\mathbf{M}} = \nabla\otimes\mathbf{U}$. From the *Lagrangean* viewpoint (1) is a coupled system of ODEs for the components of $\hat{\mathbf{a}}^{(\mathbf{2})}$. This system is closed by expressing the *4th order FO tensor* $\hat{\mathbf{a}}^{(\mathbf{4})}$ appearing on the r.h.s. of (1) as a function of $\hat{\mathbf{a}}^{(\mathbf{2})}$ by means of a *closure approximation* (see [2] for a review on this subject).

In contrast to its widespread use in numerical simulations of injection molding [1] only very little is known about the properties of the FTE. Even basic elements of a proper mathematical characterization of the FTE model, such as the description its *phase space*, are still missing at present.

Definition 1. *A real symmetric 3×3 matrix $\hat{\mathbf{a}}$ is a **FO matrix** iff it is positive semidefinite and its trace equals 1. The **phase space** $\mathcal{M}_{FT}$ of the FTE is the set of all FO matrices.*

It is of great practical importance to know exactly whether a matrix belongs to the set $\mathcal{M}_{FT}$, as the interpretability of the results of a numerical integration of the FTE requires the dependent variable $\hat{\mathbf{a}}^{(\mathbf{2})}$ to have special spectral properties during *all* steps of the calculation. By inspection of the general structure of the r.h.s. of (1) one recognizes that the equation is formally well defined for *arbitrary* real symmetric matrices. The question whether the properties of the r.h.s. of (1) automatically confine the solution trajectories to the domain $\mathcal{M}_{FT}$ can be

answered positively at least for the FTE in its *exact* form (i.e. whithout a closure approximation). However, this is no longer true if a *closure approximation* is applied, which is always necessary if one has to solve the FTE *numerically*. In this way, the problem of confinement of the solutions of the FTE to the phase space $\mathcal{M}_{FT}$ *always* arises in problems of *practical* interest.

The necessity to confine the solution of the FTE to $\mathcal{M}_{FT}$ imposes additional *constraints* on the solution that have to be taken care of during numerical integration. So the basis of any method to handle the confinement problem is a *complete description* of the phase space $\mathcal{M}_{FT}$ concerning its *topological structure* as well as its *geometry*, favourably in a *frame–invariant* way (i.e. independent of any special choice of the coordinate system). The essential parts of such a description will be presented in the following sections of this paper.

2 Basic properties and global structure of $\mathcal{M}_{FT}$

We may derive the *topological properties* of the phase space $\mathcal{M}_{FT}$ from the special properties of FO matrices (see Def. 1). Basically $\mathcal{M}_{FT}$ is a subset of the vector space of real symmetric 3×3 matrices (which is isomorphic to $\mathbb{R}^6$). Actually $\mathcal{M}_{FT}$ is a *5D* object, as the *trace condition* $\mathrm{Tr}(\widehat{\mathbf{a}}) = 1$ defines a *hyperplane* in this vector space. Although the properties of *semidefiniteness* and *unit trace* are *not* conserved for *arbitrary* linear combinations of FO matrices, they *are* conserved for *convex* ones! These basic facts are summarized in

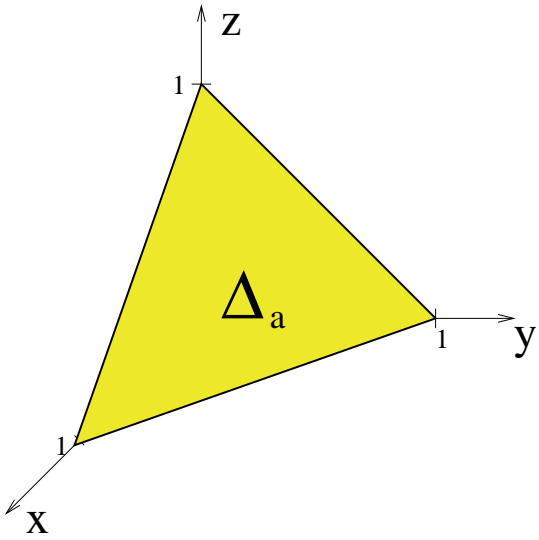
Theorem 1. *The phase space $\mathcal{M}_{FT}$ is a **bounded convex** subset of the vector space of real symmetric 3×3 matrices confined to the five–dimensional hyperplane defined by the **trace condition** $\mathrm{Tr}(\widehat{\mathbf{a}}) = 1$.*

The *convexity* of $\mathcal{M}_{FT}$ is a very useful property, as it allows for the definition of a *projection operator* onto $\mathcal{M}_{FT}$ which may be combined with any suitable ODE integrator to yield a proper integration method for the FTE (see e.g. chapter IV.4 of [3] on projection methods).

The *boundedness* of $\mathcal{M}_{FT}$ can be deduced from the *spectral representation* $\widehat{\mathbf{a}} = \sum_k \mu_k \, \mathbf{E}_k \otimes \mathbf{E}_k$ of a FO matrix in terms of its eigenvalues μ_k and eigenvectors $\mathbf{E}_k$ if *semidefiniteness* (i.e. $\mu_k \geq 0$) and the *trace condition* (i.e. $\sum_k \mu_k = 1$) are taken into account. As the elements of the orthogonal matrix diagonalizing $\widehat{\mathbf{a}}$

Figure 1

Triangle set Δ_a (see text) spanning the allowed range for the triple of diagonal elements of a FO matrix in an arbitrary coordinate system.



are given by $R_{jk} = (\mathbf{E}_k)_j$, the spectral representation in an arbitrary coordinate system can be written elementwise as $a_{ij} = \sum_k \mu_k \, R_{ik} R_{jk}$. Using $|R_{jk}| \leq 1$ we obtain the estimate $|a_{ij}| \leq 1$ for the elements of any FO matrix, which shows the boundedness of $\mathcal{M}_{FT}$. The diagonal elements $a_{jj} = \sum_k \mu_k \, R_{jk}^2$ are obviously *nonnegative* in *any* coordinate system, which confines them to the *triangle set* (see Fig. 1)

$$\Delta_a \; := \; \Big\{ (x,y,z) \in \mathbb{R}^3 \;\Big|\; 0 \leq x,y,z \leq 1 \,, \;\; x+y+z = 1 \Big\} \quad . \tag{2}$$

This provides a *necessary condition* which *invariantly* characterizes FO matrices w.r.t. their diagonal elements:

Theorem 2. *The triangle set Δ_a spans the allowed range for the triple of the diagonal elements of a FO matrix independent of the coordinate system.*

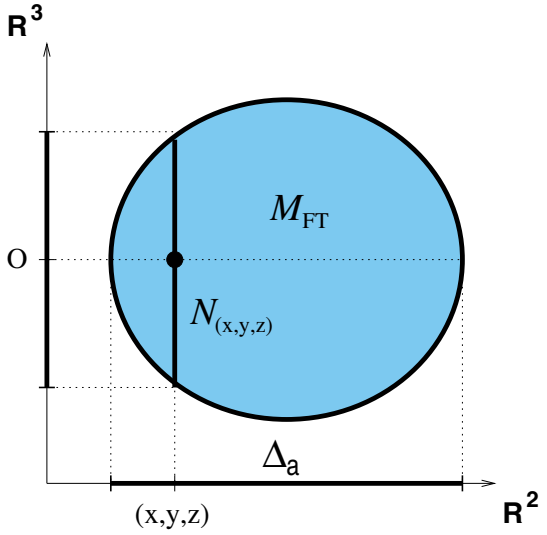
In this sense the triangle set Δ_a yields an *invariant represenation* of the "diagonal part" of the phase space $\mathcal{M}_{FT}$. Concerning the "off–diagonal part" of $\mathcal{M}_{FT}$ the situation is slightly more complicated. If we introduce the notation (x,y,z) and (u,v,w) for the triples of the *diagonal* and *off–diagonal* elements of real symmetric 3×3 matrices, we may take an arbitrary (but fixed) diagonal triple $(x,y,z) \in \Delta_a$ and formally define the set

$$\mathcal{N}_{(x,y,z)} \; := \; \Big\{ (u,v,w) \in \mathbb{R}^3 \;\Big|\; (x,y,z) \in \Delta_a \,, \; \left(\begin{smallmatrix} x & w & v \\ w & y & u \\ v & u & z \end{smallmatrix} \right) \; \in \mathcal{M}_{FT} \Big\} \tag{3}$$

of all "allowed" off–diagonal triples belonging to a fixed diagonal triple in Δ_a. This formally yields a *fibration* $\mathcal{M}_{FT} = \bigcup_{(x,y,z) \in \Delta_a} (x,y,z) \times \mathcal{N}_{(x,y,z)}$ of the phase space. The individual "fibers" $(x,y,z) \times \mathcal{N}_{(x,y,z)}$ may be regarded as locally attaching a set $\mathcal{N}_{(x,y,z)}$ of "allowed" off–diagonal triples to its "basis point"

Figure 2

Global structure of the phase space: fibration of $\mathcal{M}_{FT}$ by means of diagonal triples $(x, y, z) \in \Delta_a$ and the corresponding sets $\mathcal{N}_{(x,y,z)}$ of "allowed" off–diagonal triples



(x, y, z) chosen from Δ_a, and the variation of this basis point across the triangle set Δ_a yields a picture of the overall structure of the phase space (see Fig. 2). Although rather formal, this construction enables us to derive the essential *topological properties* of the sets $\mathcal{N}_{(x,y,z)}$:

Theorem 3. *The set $\mathcal{N}_{(x,y,z)}$ of admissible off–diagonal elements associated with a given diagonal triple $(x, y, z) \in \Delta_a$ is a **bounded convex** subset of $\mathbb{R}^3$ which contains the origin.*

Proof: As we get $(x, y, z) \times \mathcal{N}_{(x,y,z)}$ as the intersection of the two convex sets $\mathcal{M}_{FT}$ and $(x, y, z) \times \mathbb{R}^3$, we may conclude that $\mathcal{N}_{(x,y,z)}$ is also convex. As $\mathcal{M}_{FT}$ is bounded, this holds for $\mathcal{N}_{(x,y,z)}$ also. Finally a matrix consisting of any diagonal triple chosen from Δ_a and zero off–diagonal elements is a FO matrix, so each set $\mathcal{N}_{(x,y,z)}$ contains at least $(0, 0, 0)$. □

Apart from the properties of $\mathcal{N}_{(x,y,z)}$ stated in the theorem above, the visualization of the phase space $\mathcal{M}_{FT}$ provided by Fig. 2 suggests that the set $\mathcal{N}_{(x,y,z)}$ is a fully 3D object only if its "basis point" (x, y, z) is located in the interior of the triangle Δ_a and it shrinks to a single point (namely the *origin* of $\mathbb{R}^3$) on the boundary of Δ_a. In fact it can be shown (using the results of the following section) that each set $\mathcal{N}_{(x,y,z)}$ is contained within a ball of radius $R_a = \sqrt{xy + yz + zx}$ which shrinks to the origin at the *cornerpoints* of the triangle Δ_a. At the *edges* of the triangle the sets $\mathcal{N}_{(x,y,z)}$ degenerate to 1D objects: two of the off–diagonal elements are equal to zero, the third one may vary in an interval between $\pm R_a$ (see [5] for details).

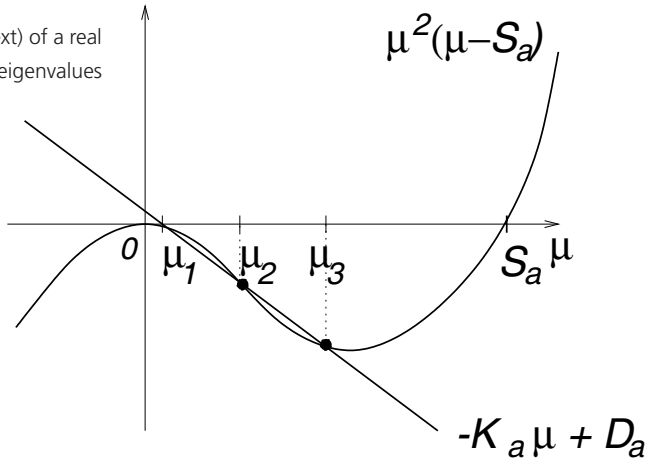


Figure 3 If the invariants S_a, K_a and D_a (see text) of a real symmetric 3×3 matrix are positive, its eigenvalues μ_k are also positive.

3 Invariant algebraic characterization of $\mathcal{M}_{FT}$

According to the results of the preceding section, a given matrix $\widehat{\mathbf{a}} = \begin{pmatrix} x & w & v \\ w & y & u \\ v & u & z \end{pmatrix}$ is a FO matrix iff its diagonal triple (x, y, z) is located on the triangle set Δ_a and its off–diagonal triple (u, v, w) belongs to the corresponding set $\mathcal{N}_{(x,y,z)}$. While the property "$(x, y, z) \in \Delta_a$" may be checked by the simple relations $x, y, z \geq 0$ and $x + y + z = 1$ defining Δ_a (see (2)), a similar characterization of the sets $\mathcal{N}_{(x,y,z)}$ by means of *invariant algebraic relations* is still missing.

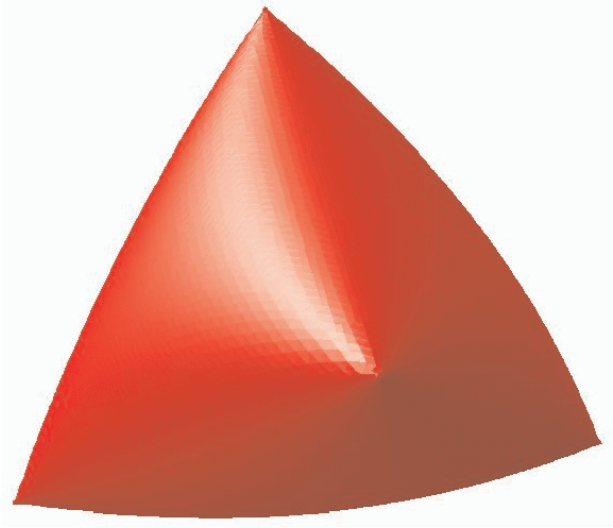
This invariant characterization may be obtained by an analysis of the *characteristic polynomial* $\det(\mu\widehat{\mathbb{1}} - \widehat{\mathbf{a}}) = \mu^2(\mu - S_a) + K_a\mu - D_a$ of a real symmetric 3×3 matrix. The coefficients $S_a = \mathrm{Tr}(\widehat{\mathbf{a}})$, $K_a = \frac{1}{2}\left[\mathrm{Tr}(\widehat{\mathbf{a}})^2 - \mathrm{Tr}(\widehat{\mathbf{a}} \cdot \widehat{\mathbf{a}})\right]$ and $D_a = \det(\widehat{\mathbf{a}})$ are simple *algebraic expressions* in the matrix elements as well as *invariants* of the matrix. Taking a look at Fig. 3 one recognizes that a *positive* trace S_a provides the existence of positive eigenvalues while *nonnegative* values of the other two invariants K_a and D_a prevent the existence of negative ones. Note that the matrix *always* has three real eigenvalues, therefore the conditions $S_a > 0$, $K_a \geq 0$ and $D_a \geq 0$ are not only *necessary* but also *sufficient* for *all* eigenvalues of $\widehat{\mathbf{a}}$ to be *nonnegative*! Combined with the trace condition $S_a = 1$, this yields the desired **invariant characterization of FO matrices**:

Theorem 4. *A real symmetric 3×3 matrix $\widehat{\mathbf{a}}$ is a **FO matrix** iff its trace S_a equals 1 and its invariants K_a and D_a are nonnegative.*

According to this theorem the set $\mathcal{N}_{(x,y,z)}$ corresponding to a given diagonal triple $(x, y, z) \in \Delta_a$ can be characterized invariantly as the set of all off–diagonal

Figure 4

In the "symmetric" case $x, y, z = \frac{1}{3}$ the set $\mathcal{N}_{(x,y,z)}$ — obtained here by plotting the algebraic inequalities $K_a \geq 0$ and $D_a \geq 0$ with **DPGraph** [4] — has the shape of an *"inflated tetrahedron"* (i.e. a tedrahedron whose edges are rounded off).



triples (u, v, w) simultaneously satisfying the pair of algebraic inequalities

$$K_a \geq 0 \quad \Leftrightarrow \quad u^2 + v^2 + w^2 \leq xy + xy + zx \ , \tag{4}$$

$$D_a \geq 0 \quad \Leftrightarrow \quad u^2 x + v^2 y + w^2 z - 2uvw \leq xyz \, . \tag{5}$$

Regarding $(u, v, w) \in \mathbb{R}^3$ as variables and $(x, y, z) \in \Delta_a$ as fixed parameters, the solution set $\mathcal{N}_{(x,y,z)}$ of the above inequalities may be plotted using suitable software (e.g. [4], see Fig. 4 for a special example).

It can be shown[2] that in general

- all sets $\mathcal{N}_{(x,y,z)}$ obtained for diagonal triples (x, y, z) chosen from the *interior* of the triangle Δ_a (i.e.: $xyz > 0$) are merely non–degenerate *deformations* of the tetrahedron–shaped "symmetric" case shown in Fig. 4,

- the *boundary* of $\mathcal{N}_{(x,y,z)}$ is the part of the hypersurface $D_a = 0$ contained within the ball given by $K_a \geq 0$, and

- this hypersurface $D_a = 0$ intersects with the sphere $K_a = 0$ at exactely four *nodal points* whose coordinates depend only on (x, y, z) and which span a *simplex* that *approximates* $\mathcal{N}_{(x,y,z)}$ from inside.

Combined with the results from the preceeding section this yields a proper view of the sets $\mathcal{N}_{(x,y,z)}$ of "allowed" off–diagonal triples in all cases and altogether completes our knowledge of the *geometry* as well as of the *topology* of the phase space $\mathcal{M}_{FT}$.

[2] The proof of the results stated above as well as further details — e.g. on the approximation of $\mathcal{M}_{FT}$ provided by the replacement of the sets $\mathcal{N}_{(x,y,z)}$ by their *approximating simplices* — may be found in [5].

4 Conclusion

The *Folgar–Tucker equation* (FTE) is used in simulations of fiber suspension flow to predict fiber orientation depending on the local velocity field of the fluid. In this paper, the essential parts of a *complete, frame–invariant description of the phase space* of the *FTE* are presented for the first time (in a rather abbreviated way). This description provides a basis for further mathematical investigations of the Folgar–Tucker model as well as for the *construction of robust numerical integration schemes* which contain the (possibly approximate) *projection on the phase space* as an integral part. Apart from beeing a useful piece of mathematics applicable to improve the numerical simulation of a widely used production process (i.e. *injection molding*) of fiber reinforced plastic parts, the investigation of the the phase space presented here reveals (in the author's view) a very nice mathematical structure which is accessible by rather simple mathematical tools.

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[5] J. Linn: *"On the phase space of the Folgar–Tucker equation"*, ITWM preprint (*in preparation*)

Published reports of the Fraunhofer ITWM

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

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

A Finite - Volume Particle Method for Compressible Flows

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

2. M. Feldmann, S. Seibold

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

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

3. Y. Ben-Haim, S. Seibold

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

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

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

Three-dimensional Radiative Heat Transfer in Glass Cooling Processes

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

5. A. Klar, R. Wegener

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

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

Part II: Numerical and stochastic investigations

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

6. A. Klar, N. Siedow

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

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

7. I. Choquet

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

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

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

Efficient Texture Analysis of Binary Images

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

9. J. Orlik

Homogenization for viscoelasticity of the integral type with aging and shrinkage

A multiphase composite with periodic distributed inclusions with a smooth boundary is considered in this contribution. The composite component materials are supposed to be linear viscoelastic and aging (of the nonconvolution integral type, for which the Laplace transform with respect to time is not effectively applicable) and are subjected to isotropic shrinkage. The free shrinkage deformation can be considered as a fictitious temperature deformation in the behavior law. The procedure presented in this paper proposes a way to determine average (effective homogenized) viscoelastic and shrinkage (temperature) composite properties and the homogenized stressfield from known properties of the components. This is done by the extension of the asymptotic homogenization technique known for pure elastic nonhomogeneous bodies to the nonhomogeneous thermoviscoelasticity of the integral noncon-

volution type. Up to now, the homogenization theory has not covered viscoelasticity of the integral type. SanchezPalencia (1980), Francfort & Suquet (1987) (see [2], [9]) have considered homogenization for viscoelasticity of the differential form and only up to the first derivative order. The integralmodeled viscoelasticity is more general then the differential one and includes almost all known differential models. The homogenization procedure is based on the construction of an asymptotic solution with respect to a period of the composite structure. This reduces the original problem to some auxiliary boundary value problems of elasticity and viscoelasticity on the unit periodic cell, of the same type as the original non-homogeneous problem. The existence and uniqueness results for such problems were obtained for kernels satisfying some constrain conditions. This is done by the extension of the Volterra integral operator theory to the Volterra operators with respect to the time, whose 1 kernels are space linear operators for any fixed time variables. Some ideas of such approach were proposed in [11] and [12], where the Volterra operators with kernels depending additionally on parameter were considered. This manuscript delivers results of the same nature for the case of the spaceoperator kernels.
(20 pages, 1998)

10. J. Mohring

Helmholtz Resonators with Large Aperture

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

11. H. W. Hamacher, A. Schöbel

On Center Cycles in Grid Graphs

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

12. H. W. Hamacher, K.-H. Küfer

Inverse radiation therapy planning - a multiple objective optimisation approach

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

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

On the Analysis of Spatial Binary Images

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

14. M. Junk

On the Construction of Discrete Equilibrium Distributions for Kinetic Schemes

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

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

A new discrete velocity method for Navier-Stokes equations

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

16. H. Neunzert

Mathematics as a Key to Key Technologies

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

17. J. Ohser, K. Sandau

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

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

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

Solving nonconvex planar location problems by finite dominating sets

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

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

19. A. Becker

A Review on Image Distortion Measures

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

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

Polyhedral Properties of the Uncapacitated Multiple Allocation Hub Location Problem

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

21. H. W. Hamacher, A. Schöbel

Design of Zone Tariff Systems in Public Transportation

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

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

The Finite-Volume-Particle Method for Conservation Laws

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

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

Location Software and Interface with GIS and Supply Chain Management

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

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

Mathematical Modelling of Evacuation Problems: A State of Art

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

25. J. Kuhnert, S. Tiwari

Grid free method for solving the Poisson equation

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

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

Simulation of the fiber spinning process

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

Keywords: Melt spinning, fiber model, Lattice Boltzmann, CFD

(19 pages, 2001)

27. A. Zemitis

On interaction of a liquid film with an obstacle

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

Keywords: impinging jets, liquid film, models, numerical solution, shape

(22 pages, 2001)

28. I. Ginzburg, K. Steiner

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

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

Keywords: Generalized LBE, free-surface phenomena, interface boundary conditions, filling processes, Bingham viscoplastic model, regularized models

(22 pages, 2001)

29. H. Neunzert

»Denn nichts ist für den Menschen als Menschen etwas wert, was er nicht mit Leidenschaft tun kann«

Vortrag anlässlich der Verleihung des Akademiepreises des Landes Rheinland-Pfalz am 21.11.2001

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

Keywords: Lehre, Forschung, angewandte Mathematik, Mehrskalenanalyse, Strömungsmechanik

(18 pages, 2001)

30. J. Kuhnert, S. Tiwari

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

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

Keywords: Incompressible Navier-Stokes equations, Meshfree method, Projection method, Particle scheme, Least squares approximation

AMS subject classification: 76D05, 76M28

(25 pages, 2001)

31. R. Korn, M. Krekel

Optimal Portfolios with Fixed Consumption or Income Streams

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

Keywords: Portfolio optimisation, stochastic control, HJB equation, discretisation of control problems.

(23 pages, 2002)

32. M. Krekel

Optimal portfolios with a loan dependent credit spread

If an investor borrows money he generally has to pay higher interest rates than he would have received, if he had put his funds on a savings account. The classical model of continuous time portfolio optimisation ignores this effect. Since there is obviously a connection between the default probability and the total percentage of wealth, which the investor is in debt, we study portfolio optimisation with a control dependent interest rate. Assuming a logarithmic and a power utility function, respectively, we prove explicit formulae of the optimal control.

Keywords: Portfolio optimisation, stochastic control, HJB equation, credit spread, log utility, power utility, non-linear wealth dynamics

(25 pages, 2002)

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

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

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

Keywords: image analysis, Euler number, neighborhod relationships, cuboidal lattice

(32 pages, 2002)

34. I. Ginzburg, K. Steiner

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

A generalized lattice Boltzmann model to simulate free-surface is constructed in both two and three dimensions. The proposed model satisfies the interfacial boundary conditions accurately. A distinctive feature of the model is that the collision processes is carried out only on the points occupied partially or fully by the fluid. To maintain a sharp interfacial front, the method includes an anti-diffusion algorithm. The unknown distribution functions at the interfacial region are constructed according to the first order Chapman-Enskog analysis. The interfacial boundary conditions are satis-

fied exactly by the coefficients in the Chapman-Enskog expansion. The distribution functions are naturally expressed in the local interfacial coordinates. The macroscopic quantities at the interface are extracted from the least-square solutions of a locally linearized system obtained from the known distribution functions. The proposed method does not require any geometric front construction and is robust for any interfacial topology. Simulation results of realistic filling process are presented: rectangular cavity in two dimensions and Hammer box, Campbell box, Sheffield box, and Motorblock in three dimensions. To enhance the stability at high Reynolds numbers, various upwind-type schemes are developed. Free-slip and no-slip boundary conditions are also discussed.
Keywords: Lattice Boltzmann models; free-surface phenomena; interface boundary conditions; filling processes; injection molding; volume of fluid method; interface boundary conditions; advection-schemes; upwind-schemes
(54 pages, 2002)

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

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

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

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

Parameter influence on the zeros of network determinants

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

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

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

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

38. D. d'Humières, I. Ginzburg

Multi-reflection boundary conditions for lattice Boltzmann models

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

39. R. Korn

Elementare Finanzmathematik

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

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

Batch Presorting Problems: Models and Complexity Results

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

41. J. Linn

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

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

42. T. Hanne, S. Nickel

A multi-objective evolutionary algorithm for scheduling and inspection planning in software development projects

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

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

Intensity-modulated radiotherapy - a large scale multi-criteria programming problem -

Radiation therapy planning is always a tight rope walk between dangerous insufficient dose in the target volume and life threatening overdosing of organs at risk. Finding ideal balances between these inherently contradictory goals challenges dosimetrists and physicians in their daily practice. Today's planning systems are typically based on a single evaluation function that measures the quality of a radiation treatment plan. Unfortunately, such a one dimensional approach cannot satisfactorily map the different backgrounds of

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

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