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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

Simulation of the fiber spinning process

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Abstract

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

Introduction

Ever since it was founded some 50 years ago, the name Neumag has conveyed the idea of continuity, experience and high quality standards in the synthetic fiber industry. Neumag's main products are engineering and manufacturing of BCF and staple fiber plants. Neumag offers contract guarantees for product quality and capacities of its plants based on full support from Neumag's engineering and R&D department.

In order to be able to give this support and for the design of new products, the simulation of the processes becomes more and more important. The main target in the design of the melt spinning process in the man-made fiber industry is to find an optimal design of the spinneret and the quench air unit for maximum throughput and best quality of the fiber produced. Depending on the process, i.e. staple fiber production or filament production, either one or the other can be more important.

How many capillaries can be put on one spinneret to achieve a maximum throughput per position? Are all filaments cooled down evenly? How long is the solidification length of the filaments? These are some of the questions arising during the design process of a spinning system.

There are several models available in the literature for simulation of the melt spinning process. Generally, a model for the fiber behavior along the spinning line is coupled with some model for the quench air flowing around the filaments. In the fiber model, the energy, momentum and mass balance are solved for the polymer mass flow coupled with a constitutive equation characterizing the polymeric material. The main difference between the different fiber models available in the literature [1-8] is this constitutive equation of the polymer.

Generally there are two approaches in modelling the quench air flow. In the first approach the actual flow of the quench air is not taken into account. The coupling of quench air and filament is accounted for by empirical equations for the temperature rise of the quench air while flowing through the filament bundle. The second approach is to model the air flow by a CFD code and then coupling the quench air and the fiber grid.

We use the second approach.

In this paper, a new model for simulation of the fiber spinning process is described which was developed by the Fraunhofer institute of applied mathematics (ITWM) in Kaiserslautern, Germany, in cooperation with Neumag GmbH & Co. KG in Neumünster, Germany. This new model is based on modelling the quench air flow as particles, thus it is called ParPac (Parallel Particle Codes) [9].

The coupling of the quench air flow field with a large number of individual filaments requires large calculation capabilities. The current installation runs on a single computer for the sake of flexibility. However, in order to save calculation time, the model includes a new algorithm for quench air simulation which can be run on parallel computers.

Method

For simulation of the melt spinning process, the calculations for the quench air flow field and the fiber cooling down in this flow field are coupled. For the simulation of the quench air flow a so-called GLB method (Generalized Lattice Boltzmann) [15, 16, 17] is used. The basic idea of this method is to model the flow as particles obeying the Boltzmann equation on a discrete grid. The GLB method is especially suited for the interaction of the fluid flow with flexible structures like filaments floating in the quench air flow. The Boltzmann equation is connected to the Navier Stokes equation in classical fluid dynamics through distribution functions representing density, velocity and temperature of the fluid flow. To quantify this connection, i.e. to calculate the respective quantities, the flow field has to be discretized.

Parallel to the calculation of the fluid flow each filament is modelled. Here, a one-dimensional model is used with grid points located along the fiber axis. The fiber itself is viewed as a viscous liquid jet, as described by A. Yarin [11,13]. It predicts the position of the fiber, i.e. its deviation in x and y direction, its cross-sectional area (f) as well as its velocity (w) and temperature (T). The properties of the fiber are assumed to be uniform across its cross section.

The energy, momentum and continuity equations are solved for the polymer mass flow coupled with a constitutive equation characterizing the polymeric material (cf. Figure 1). The momentum balance accounts for viscous forces, gravity and air drag. The energy balance accounts for convectional heat transfer and conductivity. The influence of radiation can be neglected. The three coupled second-order differential equations and the algebraic relation for the mass flux are discretized by an implicit finite difference scheme including upwinding to treat the convective terms. While solving the differential equations, also all other relevant fiber quantities, like spinning line stress etc., can be calculated.

The fiber and flow simulations have to be coupled. The coupling conditions can be derived by asymptotic methods and lead to an integral equation [14]. Since different grids are used for quench air and the filament, the results have to be interpolated between the two grids. Afterwards an iteration follows to achieve stationarity [18]. The calculation procedure is visualized in Figure 2. For a detailed description of the fiber model the reader is referred to the work of Götz [14].

Continuity equation

 $M = \rho(T(s)) \cdot w(s) \cdot f(s)$

Momentum equation

 $\frac{\partial Mw}{\partial s} = \frac{\partial}{\partial s} \left(\frac{\mu f}{\lambda} \frac{\partial w}{\partial s} \right) + F_T$

Energy equation

$$\frac{\partial cMT}{\partial s} = \frac{\partial}{\partial s} \left(\beta \frac{f}{\lambda} \frac{\partial T}{\partial s} \right) + \mu \frac{f}{\lambda} \left(\frac{\partial w}{\partial s} \right)^2 + S_T$$

Figure 1: Basic equations of the fiber model.

Experimental

To cover a wide range of fiber spinning processes, experiments were carried out with a number of polymers, different spinneret configurations and different quench air conditions. The range covered by our measurements is given in table 1.



Figure 2: Iteration scheme of the calculation method

	Monofilament	Multifilament
Polymers	PA6, PET, PP	PP
No. of filaments	1	17 to 120
No. of rows	-	1 to 12
Take off speed range [m/min]	1000 to 2000	400 to 1000
Quench air speed [m/s]	0 to 1	0 to 1
Capillary diameter [mm]	0.5	0.4
Volume flow rate per capillary [cm ³ /min]	1.5 to 2.1	0.6 to 2

Table 1: Process parameters covered by experiments

For the measurements it is important to use measurement methods which do not interfere with the process, i.e. non-contact methods. Quantities, which can be measured with non-contact methods, are the velocity and the temperature of the filament as a function of the distance from the spinneret as well as the spinning line deflection. In this work, for temperature measurements an infrared camera was used (InfraTec, Dresden, Germany) while velocity measurements were carried out using a Laser Doppler Anemometer (BSA Flowlite, Dantec, Erlangen, Germany). In some runs, the spinning line deflection was measured using two laser beams mounted on a length scale. For other quantities important in the simulation of fiber spinning processes like yarn tension or diameter, there are no reliable non-contact methods available. Figure 3 shows the test stand for temperature and velocity measurements used in the Neumag laboratory.

Figure 4 shows a typical result of a velocity measurement with the LDA. One can clearly see the peak at 8.3 m/s even though the filament moves in the quench air flow and cannot be focussed within the measurement volume of the instrument at all times.

Figure 5 shows the infrared image of a single filament at approx. 140°C. Since also in temperature measurement, the filament cannot be focussed by the camera at all times, we took 300 IR-images during each run. The highest temperature occurring in these images was taken to be the yarn temperature. An estimate on the Biot number of the heat transfer from the filament to the quench air shows that the filament temperature is essentially uniform across its cross-section.



Figure 3: Test stand for velocity and temperature measurement: Infrared Camera and Laser Doppler Anemometer



Figure 4: Result of velocity measurement with the Laser Doppler Anemometer



Figure 5: Infrared image of a single filament having a temperature of approximately 140 °C

Figure 6 shows the measured quench air profile and spinning line deflection for a PP filament at quench air speed v = 0.8 m/s. In Figure 7 and Figure 8 the measured temperature and velocity profiles of a PP Monofilament for different quench air speeds are shown.



Figure 6: Measured quench air profile and spinning line deflection of a PP Filament.



Figure 7: Measured temperature profiles of a PP monofilament at different quench air speeds (0 m/s, 0.5 m/s, 1 m/s).



Figure 8: Measured velocity profiles of a PP monofilament at different quench air speeds (0 m/s, 0.5 m/s, 1 m/s).

Comparison of Simulations and Experiments

Simulations were carried out for the process parameters used in the experiments in order to compare the results. The material model parameters were fitted to the experimental results of velocity and temperature profiles of the monofilaments of the different polymers.

Figure 9 shows simulations and experimental results of the temperature profile of the last row of polypropylene (PP) multifilaments from different spinnerets. Simulations and experiments agree well within the experimental uncertainties. Only at lower temperatures around 50°C can one see larger deviations, which are at the lower end of the working range (50 to 300°C) of the IR camera in the configuration used here. Experiments as well as simulations show the influence of the number of rows on the temperature profile. The difference in the temperature profile between the two spinnerets with 12 rows is due to two effects. First, the experiments with the spinnerets with shifted rows were run with a quench air speed of 0.8 m/s, while the experiments with straight rows were run at 0.5 m/s. Secondly, the shifted rows allow a better cooling of each filament.

Figure 10 shows simulated and experimental velocity profiles of PP multifilaments from spinnerets with one and two rows. The simulation results can predict the influence of the number of rows very well. Also, the point of solidification is predicted well by the model. Only the slope of the velocity profile is larger in simulation results than in experiments. The reason for this lies within the fiber model of the simulation procedure. We are currently improving the fiber model to meet the experimental data more precisely.

Figure 11 shows the simulated temperature and velocity profiles for a PET Monofilament. The material parameters of the model were determined from measurements under different process conditions. Agreement between simulation and experiment also for this material is very good for the velocity profile. Larger deviations can be seen in the temperature profile.

The quality of the model can also be seen in Figure 12, where the spinning line deflection calculated by the model and experimental data are compared for PP filaments. The agreement between simulation and experiment is very good.



Figure 9: Simulated and experimental temperature profiles for different spinneret configurations, 6 rows and 12 rows (straight and shifted).



Figure 10: Simulated and experimental velocity profiles for different spinneret configurations, 1 row and 2 rows.



Figure 11: Simulated and experimental temperature and velocity profile of a PET monofilament.



Figure 12: Calculated and measured spinning line deflection of PP filaments.

Conclusion

The ParPac (**Par**allel **Pa**rticle **C**ode) Program, uses the Lattice Boltzmann method to calculate the quench air flow and couple it to a fiber model. It enables us to simulate the influence of all process parameters of the melt spinning process with different hole configurations. Thus, the design of such processes can be optimized.

The layout of the spinneret, i.e. the number of holes, the number of rows and the distances between each hole, can be exactly matched to the process requirements. Process parameters can be chosen to yield the desired product qualities. The model parameters were determined from measurements with monofilaments of PP, PET and PA6. The simulation results were then validated by comparing them with experimental data for multifilaments from spinnerets with different configurations. Agreement between simulations and experiments is generally very good.

Acknowledgments

The authors are grateful to the BMBF for the financial support of the project under grant nr. 01 IR 801 C. Especially the support of the project coordinator Dr. R. Krahl from Deutsches Zentrum für Luft- und Raumfahrt e.V. is gratefully acknowledged.

Symbols

	unit	Description
Т	К	temperature
W	m/s	fiber velocity
r	m	radius
f	m ²	area
Μ	kg/s	mass flux
S	m	coordinate along fiber axis
\mathbf{F}_{T}	Ν	sum of gravitational and drag forces
S_{T}	W/m	heat exchange with surrounding air
С	J/kg K	specific heat
Н	m	deflection of fiber
	kg/m³	Density
	m²/s	kinematic viscosity
		extension of fiber (see [Goetz])

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Bisher erschienene Berichte des Fraunhofer ITWM

Die PDF-Files der folgenden Berichte finden Sie unter: www.itwm.fhg.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 S., 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 signalbased 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 nonlinearities 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 S., 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 multihypothesis 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, multihypothesis diagnosis, rotating machinery, crack diagnosis (24 S., 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 S., 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 S., 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 S., 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 S., 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 Eley-Rideal and Langmuir-Hinshelwood 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 S., 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 S., 1998)

9. J. Orlik

Homogenization for viscoelasticity of the integral type with aging and shrinkage

A multi-phase 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 stress-field from known properties of the components. This is done by the extension of the asymptotic homogenization technique known for pure elastic non-homogeneous bodies to the non-homogeneous thermo-viscoelasticity of the integral non-convolution type. Up to now, the homogenization theory has not covered viscoelasticity of the integral type.

Sanchez-Palencia (1980), Francfort & Suguet (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 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 space-operator kernels. (20 S., 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. (21 S., 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 S., 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 trialand-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 5., 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 5., 1999)

20 5., 1555,

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 S., 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 S. 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 S. (vier 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 S., 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 S., 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 S., 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 facetdefining. We show its superior computational performance by benchmarking it on a well known data set. Kevwords:

integer programming, hub location, facility location, valid inequalities, facets, branch and cut (21 S., 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 S., 2001)

22. D. Hietel, M. Junk, R. Keck, D. Teleaga: The Finite-Volume-Particle Method for **Conservation Laws**

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

After a brief derivation of the Finite-Volume-Particle Method, this work focuses on the role of the geometric coefficients in the scheme (16 S., 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

Kevwords

facility location, software development, geographical information systems, supply chain management. (48 S., 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 guickest 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 S., 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 S., 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 S., 2001)