



Fraunhofer Institut
Techno- und
Wirtschaftsmathematik

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Parallel lattice Boltzmann simulation
of complex flows

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ISSN 1434-9973

Bericht 61 (2004)

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Vorwort

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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

Parallel lattice Boltzmann simulation of complex flows

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Summary:

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

Keywords:

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

1 Introduction

Lattice Boltzmann methods are relatively new and quite popular numerical schemes for solving the incompressible Navier-Stokes equations of mathematical fluid dynamics in a very special way. Unlike conventional Navier-Stokes solvers, they do not approximate the equations directly but simulate fluid behaviour on a mesoscopic level and determine pressure and velocity by calculating certain moments of the particle density. The main advantages of lattice Boltzmann methods are the relative simplicity of the underlying mesoscopic equations in comparison to Navier-Stokes and their property of providing not only pressure and velocity but also the gradient of the velocity field. In practice, especially the possibility to describe boundary conditions in a very simple yet robust way, their outstanding eligibility for parallelisation, and the possibility of obtaining the velocity gradient without numerical differentiation make them very attractive.

The aim of the present paper is to demonstrate that lattice Boltzmann methods have in fact proven their capability of solving some practically relevant problems in a very convincing way. For this purpose, after a short introduction to the basic concepts of lattice Boltzmann methods in Section 2 and a brief description of the Hardware currently used by the author in Section 3, Section 4 explains the ideas of virtual material design and, especially, the role of lattice Boltzmann simulations in this field. Section 5 deals with theory and application of lattice Boltzmann algorithms for simulating pseudo-plastic fluids, and Section 6 describes a recent industrially relevant project involving lattice Boltzmann simulations of pseudo-plastic flow in microstructures. Finally, Section 7 concludes the paper and gives some rough ideas on what the future of lattice Boltzmann simulation might look like.

2 Lattice Boltzmann methods

Lattice Boltzmann methods [15, 21] are special numerical schemes for solving the incompressible Navier-Stokes equations [1, 8],

$$\operatorname{div} \mathbf{u} = 0 \quad \text{and} \quad \partial_t(\rho \mathbf{u}) + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \mu \Delta \mathbf{u},$$

where \mathbf{u} stands for the fluid velocity, ρ represents density, p denotes pressure, μ represents viscosity, and \otimes stands for the tensor product of two vectors. Fluids fulfilling those equations for a constant viscosity are called Newtonian, all others are referred to as non-Newtonian.

In lattice Boltzmann methods, instead of discretising the Navier-Stokes equations directly we simulate particle dynamics on a mesoscopic scale. For this purpose we discretise the computational domain using a regular lattice with equidistant nodes. At each time t , we consider the particle density $f(t, \mathbf{x}; \mathbf{v})$ located lattice node \mathbf{x} and moving with lattice velocity \mathbf{v} , where \mathbf{v} can only take certain constant values that make sure the particle density is moving from one lattice point to another during one time step. As an example, the possible values of \mathbf{v} for the so-called D2Q9 model in two space dimensions with nine possible lattice velocities are visualised in Fig. 1.

The lattice Boltzmann equation takes the form [17]

$$f(t + \delta t, \mathbf{x} + \mathbf{v} \delta t; \mathbf{v}) = f(t, \mathbf{x}; \mathbf{v}) + \mathbf{Q}(f)(t, \mathbf{x}; \mathbf{v}),$$

where \mathbf{Q} represents the so-called collision operator. There are several possibilities to choose the collision operator, each of them defining a special lattice Boltzmann scheme. Note that by properly choosing the collision operator, it is also possible to set up a lattice Boltzmann scheme for simulating Stokes flow instead of Navier-Stokes flow. In any case, the macroscopic quantities p and \mathbf{u} are obtained via averaging,

$$p(t, \mathbf{x}) = c_s^2 \sum_{\mathbf{v}} f(t, \mathbf{x}; \mathbf{v}) \quad \text{and} \quad \mathbf{u}(t, \mathbf{x}) = \frac{\sum_{\mathbf{v}} \mathbf{v} f(t, \mathbf{x}; \mathbf{v})}{\sum_{\mathbf{v}} f(t, \mathbf{x}; \mathbf{v})}$$

with a lattice dependent constant c_s^2 . The tuple (p, \mathbf{u}) is then an approximation of first order in time of the macroscopic (Navier-)Stokes equations. This can be shown by three different approaches, namely by Chapman-Enskog-Analysis [9], equivalent moment analysis [13], or direct asymptotic analysis [14].

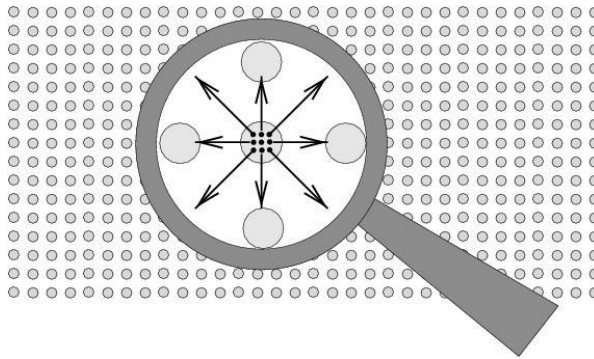


Fig. 1: In the D2Q9 model, the lattice velocity can correspond to the zero vector, to a vector pointing to a neighbouring node in a lattice direction, or to a vector pointing to a neighbouring node in diagonal direction.

3 Hardware description

The parallel computer currently used at Fraunhofer ITWM is a Linux cluster with distributed memory, manufactured by LinuxNetworkx and consisting of a login node, a management node, and 64 compute nodes. All compute nodes are equipped with two 2.4 GHz Intel® Xeon™ processors, 4 GB RAM, and 80 GB hard disk space. The login node also has two 2.4 GHz Intel® Xeon™ processors, while the management node is powered by two Intel® Pentium® III CPUs.

4 Virtual material design

In this section, the ideas of virtual material design are exemplified for the determination of an important characteristic of porous materials, namely the so-called permeability tensor. Heuristically spoken, this tensor measures the influence of the material on Newtonian flow through its pores. Its determination splits up into providing a geometrical model of the microstructure of the porous material (Section 4.1) and the computation of the tensor components by lattice Boltzmann simulation of fluid flow in this microstructure model (Section 4.2).

4.1 Microstructure modelling

Here, two main approaches for obtaining a geometric model of the microstructure of a porous material are described: The detailed analysis of a given material by the use of synchrotron tomography, i.e. by exposing a material probe to X-rays from different angles and reconstructing its microstructure from its absorbing behaviour, and the construction of a virtual microstructure from some basic material properties, like solid volume fraction and anisotropy.

Synchrotron tomography is an expensive but very reliable procedure for analysing the microstructure of a given material. It directly yields a highly resolved computer model of the microstructure of the considered material sample, only occasionally it is necessary to filter out some artefacts. However, due to memory restrictions even on modern parallel hardware, calculations are typically performed only in a cut-out of the original model. Fig. 2 shows a 2d cut through such a microstructure model, an image of a virtual material sample extracted from the same model, and a picture of that section of the virtual sample which was finally used to perform computations.

It is also possible to create virtual material samples directly using Fraunhofer ITWM's software tool GeoDict [10]. Starting from some basic geometric input parameters like solid volume fraction or the desired anisotropy, GeoDict constructs a virtual material sample of cuboidal shape, as exemplified in Fig. 3. Even though the tool was originally designed for producing virtual microstructures of non-woven textiles, it is also capable of modelling other types of porous material.

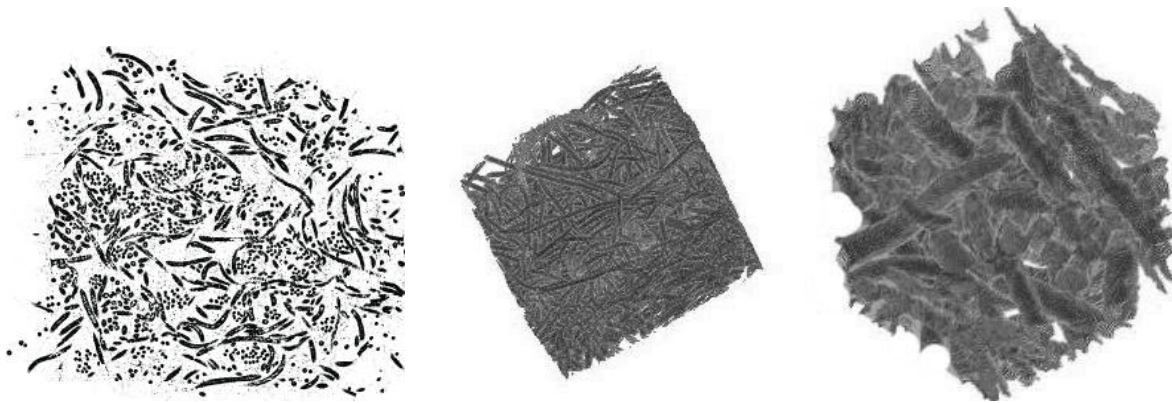


Fig. 2: A cut through a virtual sample of a non-woven textile as obtained by synchrotron tomography (left, edges: 4 mm resp. 1024 voxels), a 3d geometry extracted from this virtual sample (centre, long edge: 2 mm resp. 512 voxels), and an extract from the 3d geometry that was used for CFD simulations (right, edges: 0.5 mm resp. 128 voxels)

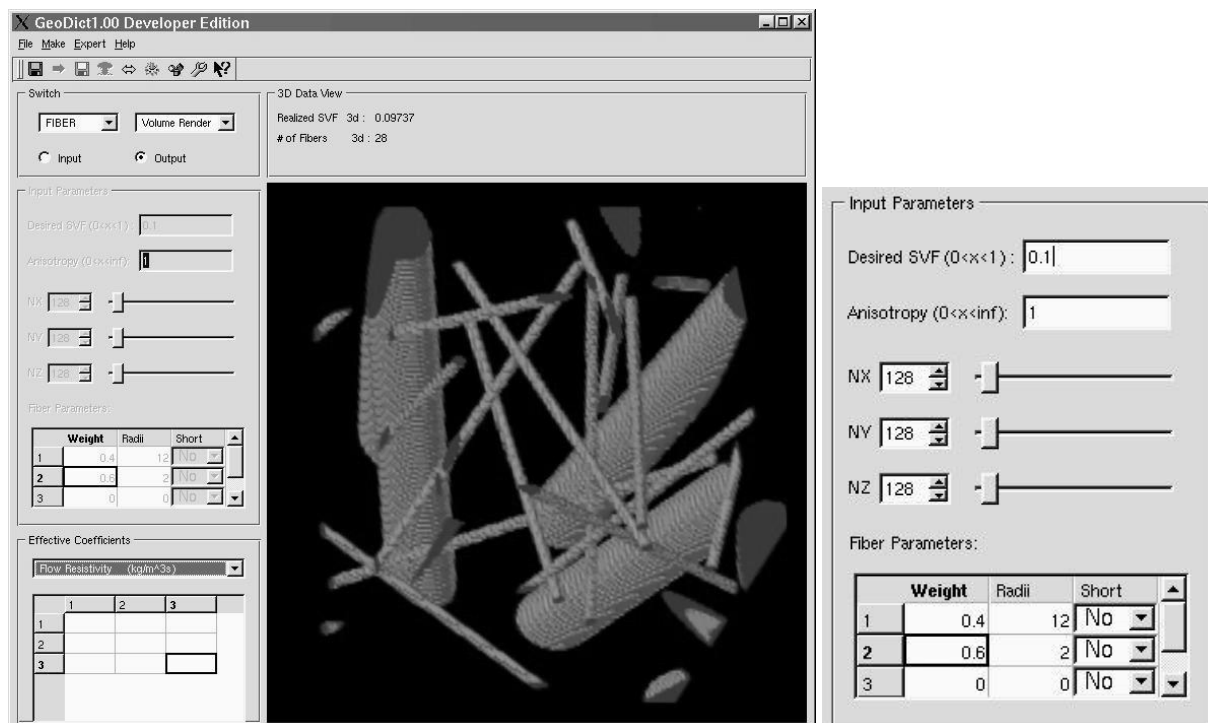


Fig. 3: Screenshot of the GeoDict GUI (left) and of the input parameters lead to the fibre geometry in the graphics window (right)

4.2 Calculation of material parameters

In the following, the calculation of material parameters shall be exemplified by the determination of the flow permeability of a given virtual material. For convenience, we assume that the edges of the sample are parallel to the cartesian coordinate axes. The mathematical basis of this procedure is Darcy's law for flow in porous media [6, 18],

$$\bar{\mathbf{u}} = -\frac{1}{\mu} \mathbf{K} \text{grad } p,$$

where $\bar{\mathbf{u}}$ denotes the average flow velocity and \mathbf{K} represents the permeability tensor of the porous medium. The component k_{ij} of the permeability tensor represents the permeability of the material in the direction parallel to the j^{th} coordinate axis if the main flow direction is parallel to the i^{th} coordinate axis. As a direct consequence, the off-diagonal elements of \mathbf{K} are equal to zero. Furthermore, if the

pressure gradient and, therefore, the main flow direction are parallel to the i^{th} coordinate axis, Darcy's law reduces to the scalar equation

$$\bar{u}_i = -\frac{k_{ii}}{\mu L} \delta p, \quad \text{which can be rewritten in the form} \quad k_{ii} = -\frac{\mu L \bar{u}_i}{\delta p}.$$

Above, \bar{u}_i is the average flow speed, L represents the length of that edge of the sample which is parallel to the i^{th} coordinate axis, and δp stands for the pressure drop parallel to the i^{th} coordinate axis. The present situation is visualised in Fig. 5.

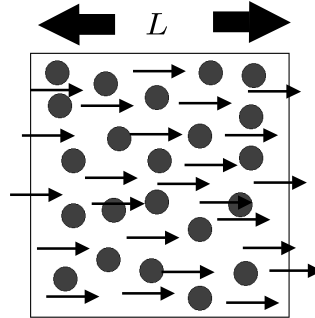


Fig. 5: A 2d porous medium, main flow direction from left to right, the edges parallel to the main flow direction have length L

Now, we choose appropriate values for μ as well as δp and determine \bar{u}_i for $i=1,2,3$ by solving the Stokes equations. Note that the Stokes equations are used here instead of the Navier-Stokes equations because Darcy's law is based on Stokes flow and not on Navier-Stokes flow [18]. Finally, we calculate the diagonal components of the permeability tensor using the scalar version of Darcy's law. Since the off-diagonal components are zero anyway, the tensor is now fully determined. Note here that in the special case of a completely isotropic material, permeability reduces to a scalar value.

In case the permeability computed by the above procedure is not satisfactory, the whole procedure may be repeated for a modified microstructure. By iterating this procedure for several times it is possible to considerably improve the virtual material in the sense of bringing its permeability closer to the theoretical optimum for a given purpose.

5 Simulation of pseudo-plastic fluids

The aim of the present Section is to introduce the modelling of a special type of non-Newtonian fluids, the so-called pseudo-plastic fluids, and to demonstrate the very natural and specifically robust treatment of such fluids by lattice Boltzmann algorithms. In particular, Section 5.1 introduces a mathematical model of pseudo-plastic fluids and Section 5.2 presents some numerical results for a simple model problem.

5.1 Theoretical background

It has been found by experiments that for many fluids, the viscosity μ is not a constant but a linearly decreasing function of the shear rate

$$\dot{\gamma} = \sqrt{\frac{1}{2} (\text{grad } \mathbf{u} + (\text{grad } \mathbf{u})^T) : (\text{grad } \mathbf{u} + (\text{grad } \mathbf{u})^T)},$$

tending to some limit μ_∞ for $\dot{\gamma} \rightarrow \infty$ [19], as exemplified in Fig. 6. Those fluids are referred to as pseudo-plastic or shear-thinning. Note that the pseudo-plastic effect typically occurs over several orders of magnitude.

The main difficulty in modelling pseudo-plastic fluids is the calculation of the shear-rate, in particular the determination of the velocity gradient. While most numerical methods for simulating fluid flow depend on numerical differentiation, which is in general unstable, for obtaining velocity gradients, lattice Boltzmann schemes offer a more elegant and very stable approach [11]. This approach is sketched in the following paragraph.

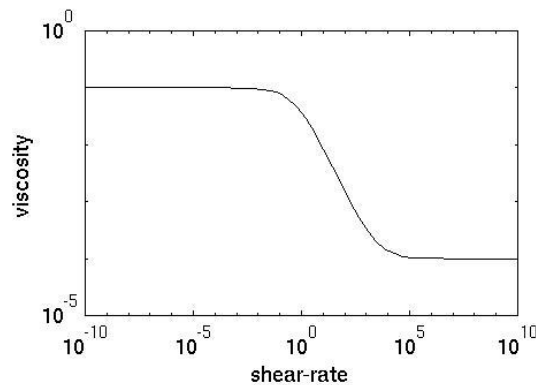


Fig. 6: Typical viscosity of a pseudo-plastic fluid versus the shear-rate

One of the basic ideas of Chapman-Enskog-Analysis [9] is to write the particle density f in the form

$$f = f^{eq} + \varepsilon f^{(1)} + \varepsilon^2 f^{(2)} + O(\varepsilon^3)$$

with a known function f^{eq} and a small parameter ε . After a lengthy calculation, it turns out that

$$\varepsilon f^{(1)}(r, \mathbf{x}; \mathbf{v}) = \frac{1}{\lambda} \text{grad}(\rho \mathbf{u})(t, \mathbf{x}) : \mathbf{W}(\mathbf{v}) + O(\varepsilon^2),$$

where λ is a known constant and $\mathbf{W}(\mathbf{v})$ is a known matrix. Since \mathbf{v} can only take values from a finite discrete set, this equation can be interpreted as a vector equation in which each value of \mathbf{v} determines one component. Approximating the vector $\varepsilon f^{(1)}(t, \mathbf{x})$ by $\mathbf{f}(t, \mathbf{x}) - f^{eq}(t, \mathbf{x})$, projecting the result on a properly chosen set of basis vectors, and finally performing some basic algebra leads to the components of the matrix $\text{grad} \mathbf{u} + (\text{grad} \mathbf{u})^T$. At this stage, the shear-rate can be determined by direct calculation.

Once the shear rate is known, it is possible to model pseudo-plastic effects. From the miscellaneous approaches that are known [19], the Cross model [5]

$$\mu(\dot{\gamma}) = \mu_\infty + \frac{\mu_0 - \mu_\infty}{1 + (C\dot{\gamma})^m}$$

where $\mu_\infty = \lim_{\dot{\gamma} \rightarrow \infty} \mu(\dot{\gamma})$ and $\mu_0 = \mu(0)$ while C and m are material-dependent constants, was chosen for the simulations described in the following.

5.2 Channel flow

The aim of this Section is to demonstrate the difference between pseudo-plastic fluids and fluids with constant viscosity. For this purpose, the flow of an artificial pseudo-plastic fluid with

$$\mu(\dot{\gamma}) = 0.0001 + \frac{0.01 - 0.0001}{1 + (80\dot{\gamma})^{1.3}} \text{ Pa} \cdot \text{s}$$

is compared to an artificial Newtonian fluid with $\mu = 0.001 \text{ Pa} \cdot \text{s}$. The benchmark considered here is flow through a 2d rectangular channel with solid boundaries at top and bottom and periodic boundaries at left and right. Initially, the fluid is at rest, and a constant force of $1000 \text{ N} / \text{m}^3$ pointing from left to

right is applied to induce the flow. Fig. 7 shows the velocity profile of both fluids at stationary state, Fig. 8 displays shear-rate and viscosity of the pseudo-plastic one at stationary state. While the Newtonian fluid exhibits the well-known parabolic velocity profile, the corresponding curve for the pseudo-plastic case is flattened around its maximum. Roughly spoken, the reason why this happens is the following: The shear-rate is equal to zero at the maximum of the velocity profile and is monotonously increasing towards the solid boundaries. Therefore, the viscosity has its maximum at the same position as the flow speed, i.e. in the centre of the channel, and is monotonously decreasing towards the solid boundaries. This behaviour of the viscosity allows the flow to speed up away from the centre of the channel. Note here that the no-slip conditions at the solid boundaries are not affected by this effect.

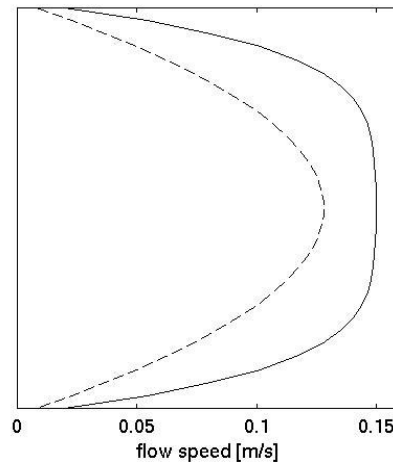


Fig. 7: Velocity profiles for pseudo-plastic (solid line) and Newtonian (dashed line) flow in a rectangular 2d channel. Note that the solid boundary at top and bottom are located slightly beyond the plotted domain.

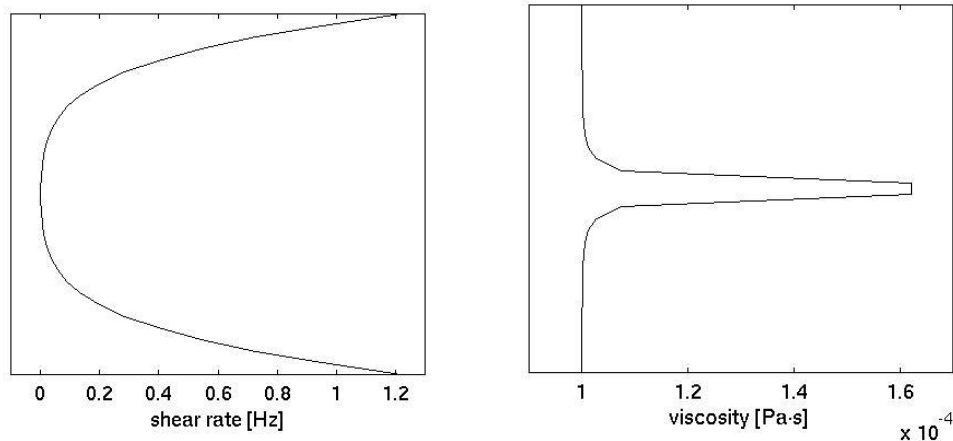


Fig. 8: Shear-rate (left) and viscosity (right) of a pseudo-plastic fluid flowing through a rectangular 2d channel at stationary state

6 Liquid composite moulding (LCM)

In the present Section, some results from a joint project of Fraunhofer ITWM and Institut für Verbundwerkstoffe GmbH (IVW), Kaiserslautern, Germany, are presented. The aim of this project is to model the injection of in-situ polymerising polyamides in beds of carbon fibres, and to simulate their flow, where in-situ polymerising means the polyamides have already started to solidify when they are injected to the fibre bed. A deep understanding of this process yields a definite improvement in designing new carbon fibre reinforced plastic materials.

The simulations performed in this project are based on experiments done with the apparatus shown in Fig. 9. Two physical scales are being considered to simulate the flow in the fibre bed: A macroscopic one, where the whole fibre bed is considered a porous medium and a Darcy-like equation is set up to

simulate the Flow [4], and a microscopic one, where the fibre geometry is resolved and a lattice Boltzmann algorithm is used to simulate the flow inside. The latter is necessary to obtain a generalisation of the permeability tensor for flow of pseudo-plastic fluids on which the macroscopic Darcy-like equation can be based. In the following, the simulation procedure on the microscopic level is described in detail.

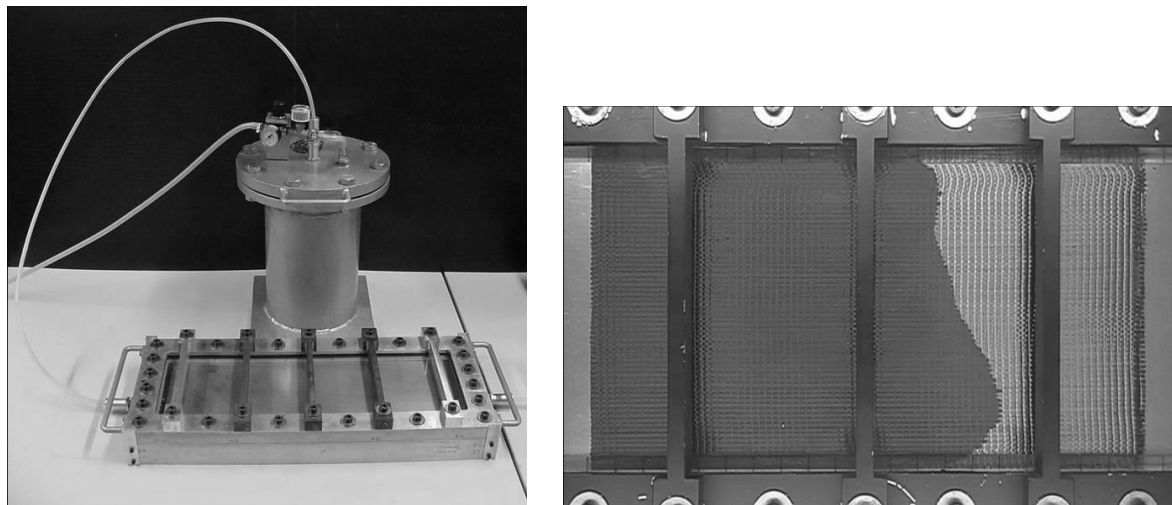


Fig. 9: The experimental apparatus used in the LCM project: The whole device consisting of the strictly fixed fibre bed, the liquid reservoir, and a system of flexible tubes (left), as well as a top view of the half saturated fibre bed (right), where the flow front is clearly visible.

In order to arrange a computer model of the flow channel, a solidified material sample produced in a laboratory experiment is cut along a line perpendicular to the flow direction, and highly resolved images of the cutting area are taken. Those images are then de-noised and extended to 3d space. Fig. 10 and 11 show a lowly resolved grinding image of the whole fibre bed and a highly resolved grinding surface image of a small cut-out, respectively, together with virtual grinding surface images of the resulting flow geometries.

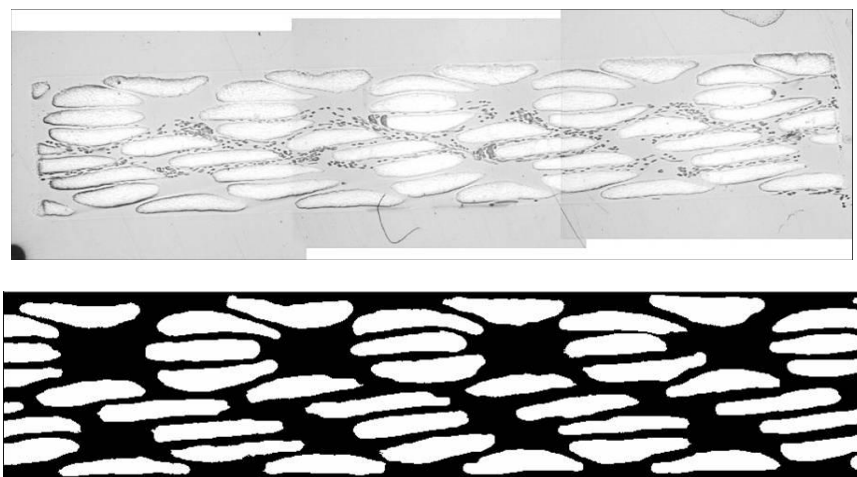


Fig. 10: Lowly resolved grinding surface image of the fibre bed (top), where the bright spots mark the fibre bundles and the dark spots mark some air bubbles enclosed in the material probe, together with the resulting digital model of the flow channel (bottom), where white marks the fibre bundles and black marks the flow channel. The lattice size is 1024 x 224 x 6.

The fluid under investigation is the epoxy resin Ly 113 / Hy 97, which is polymerising due to a chemical reaction. The shear-dependent viscosity of the liquid at different time intervals after the start of the chemical reaction is represented by the Cross models shown in Fig. 12, which are based on measurements by M. Repsch of IVW. In the following, the viscosity function for $t = 4800$ s, i.e.

$$\mu(\dot{\gamma}) = 1.2 + \frac{500 - 1.2}{1 + (80\dot{\gamma})^{1.3}} \text{ Pa} \cdot \text{s} ,$$

is exclusively used to represent Ly 113 / Hy 97, and the Newtonian fluid it is compared with has always the viscosity $\mu = 15.32 \text{ Pa} \cdot \text{s}$.

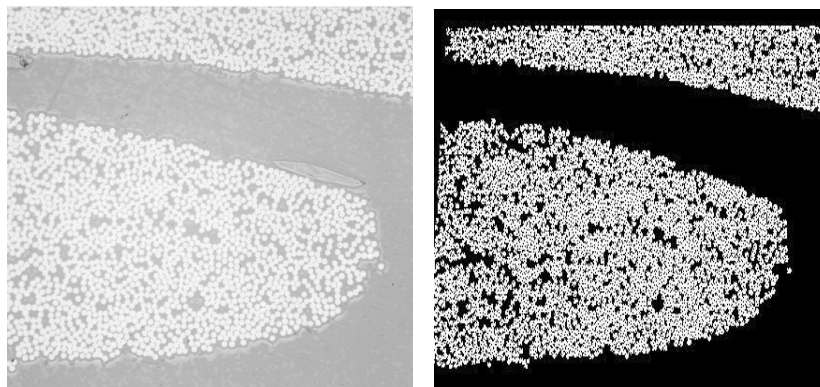


Fig. 11: Highly resolved grinding surface image of a small cut-out of the fibre bed (left), where the bright spots mark the fibres and the dark spot marks an air bubble enclosed in the material probe, together with the resulting digital model of the flow channel (right), where white marks the fibres and black marks the flow channel. The lattice size is $1024 \times 1024 \times 6$.

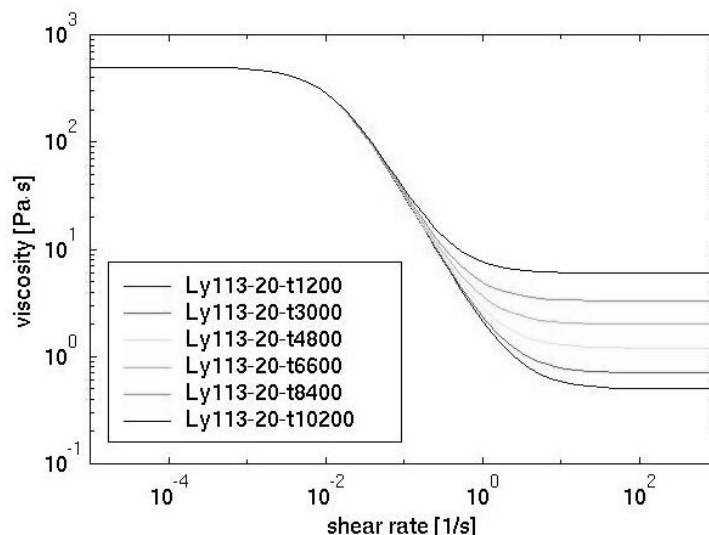


Fig. 12: Cross models for the viscosity function of Ly 113 / Hy 97 at different time intervals after the start of the solidification. The functions are based on measurements done by M. Repsch of IVW.

As visualised in Fig. 13, the flow between the single fibres inside a fibre bundle is negligible compared to the flow in the channels between the fibre bundles. Therefore, the flow channel displayed in Fig. 10 can be used for the simulation and it is not necessary to resolve the single fibres. Note that simulating the whole fibre bed with all fibres resolved is impossible anyway, even on modern parallel hardware like the Linux cluster described in Section 3, because of the enormous amount of data that had to be processed. A comparison of flow fields for Ly 113 / Hy 97 and a Newtonian fluid is given in Fig. 14, and a corresponding plot of average flow speed vs. pressure drop is given in Fig. 15.

On eight nodes (i.e. 16 processors) of the Linux Cluster described in Section 3, it takes slightly more than one hour in the Newtonian case and a bit more than six hours in the pseudo-plastic case to compute the results visualised in Fig. 13 (lattice: $1024 \times 224 \times 6$). The results shown in Fig. 14 (lattice: $1024 \times 1024 \times 6$) need about three days in the Newtonian case and approximately one week in the pseudo-plastic case on the same number of nodes on the same machine. Note that these values can only give a rough idea on simulation costs since computing time also heavily depends on some input parameters, e.g. the magnitude of the driving force.

It is left for future work to replace the extended 2d geometries by real 3d microstructures and to simulate the behaviour of the flow front during infiltration.

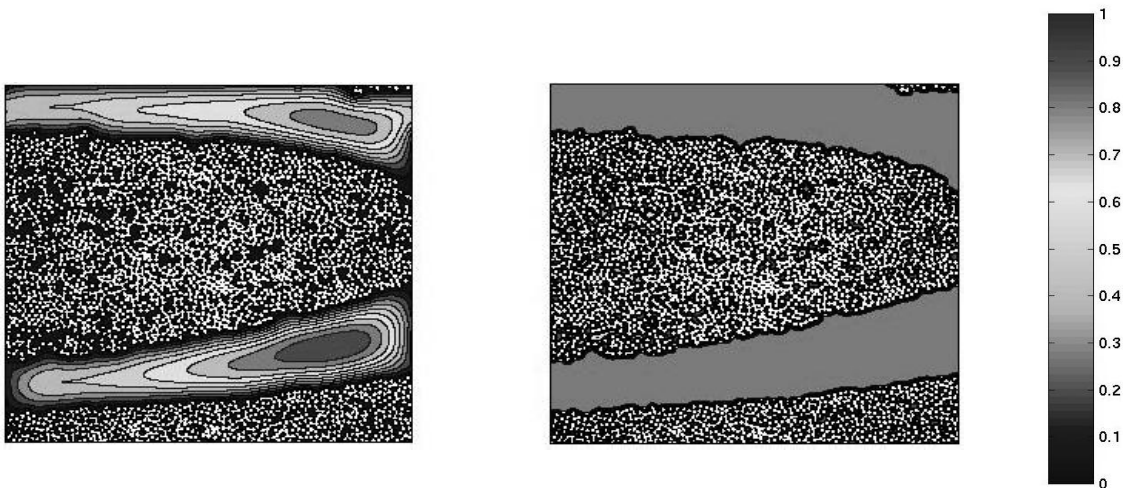


Fig. 13: Dimensionless velocity field (in u / u_{\max}) for the flow of a Newtonian (left) and a pseudo-plastic (right) fluid in the geometry from Fig. 11. For both fluids, the flow inside the fibre bundles is negligible compared to the flow outside the fibre bundles.

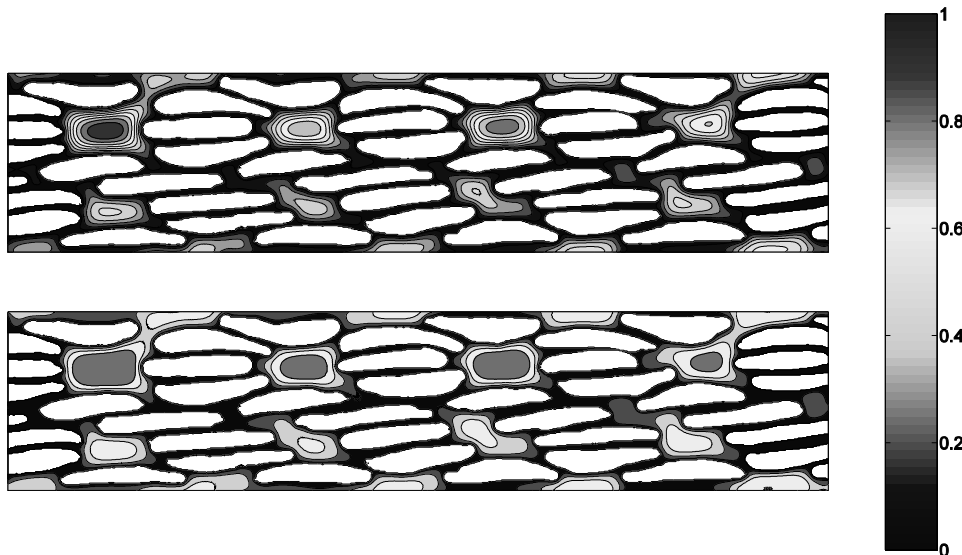


Fig. 14: Dimensionless velocity field (in u / u_{\max}) for the flow of a Newtonian (top) and a pseudo-plastic (bottom) fluid in the geometry from Fig. 10.

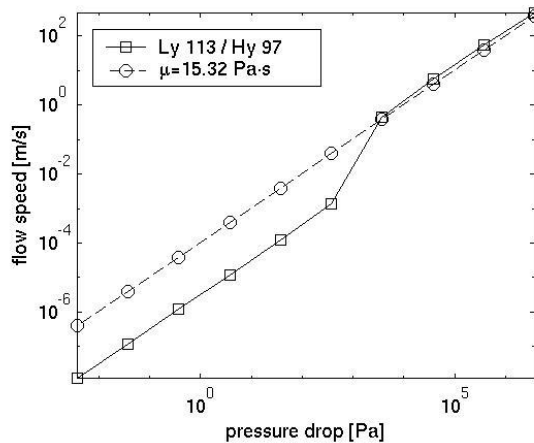


Fig. 15: Flow speed vs. pressure drop for Ly 113 / Hy 97 and a Newtonian fluid

7 Concluding remarks

After a short introduction to lattice Boltzmann algorithms and a brief description of a modern parallel computer capable of performing 3d lattice Boltzmann simulations of industrially relevant problems, the principles of realistic microstructure simulation and the applicability of lattice Boltzmann methods in this field were considered. Thereafter, a typical mathematical model of pseudo-plastic fluids was introduced and the very natural and extremely robust way in which lattice Boltzmann methods are able to handle such a model was explained and exemplified by numerical results for channel flow. Finally, a recent industrially relevant project involving lattice Boltzmann simulations of pseudo-plastic fluid flow in microstructures was dealt with. Microstructure simulation and computations for pseudo-plastic fluids are two fields where lattice Boltzmann methods have clearly proven their practical usability for industrially relevant problems and, especially in the latter case, their ability to compete with other numerical methods for simulating fluid flow.

Compared to finite volume or finite element schemes, lattice Boltzmann methods are very young, and many questions are still open. The most prominent fields of research are probably the accurate simulation of physical two-phase [15] and moving boundary [3, 12, 16] flow, the advanced treatment of boundary conditions [2, 12, 14, 22], the exploitation of the special properties of lattice Boltzmann schemes for simulating turbulence [21], and the introduction of adaptive lattice refinement [7, 20]. Thus, there is a great potential for further improvement or development of ideas from which other methods may benefit as well.

In summary, it is already reasonable to use lattice Boltzmann methods for some special fields of application, and it is definitely worthwhile to further investigate them.

8 Acknowledgements

Much of the author's research on lattice Boltzmann methods was funded by the Deutsche Forschungsgemeinschaft (German Research Council) via the projects "Analyse von Lattice-Boltzmann-Methoden" and "LBE für freie Randwertprobleme und Mehrphasenströmung". Furthermore, the author thanks A. Latz (Fraunhofer ITWM) for many valuable discussions on how to model non-Newtonian fluids and A. Wiegmann (Fraunhofer ITWM) for providing GeoDict.

The work done by U. Huber, M. Repsch (both IVW), O. Iliev, S. Rief, K. Steiner (all Fraunhofer ITWM), and R. Ciegis (TU Vilnius, during a stay at Fraunhofer ITWM) for the LCM project is highly appreciated. Also the funding of the same project by the Deutsche Forschungsgemeinschaft is gratefully acknowledged.

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

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

A Finite - Volume Particle Method for Compressible Flows

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

2. M. Feldmann, S. Seibold

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

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

Keywords: Hilbert transform, damage diagnosis, Kalman filtering, non-linear dynamics
(23 pages, 1998)

3. Y. Ben-Haim, S. Seibold

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

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

Keywords: Robust reliability, convex models, Kalman filtering, multi-hypothesis diagnosis, rotating machinery, crack diagnosis
(24 pages, 1998)

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

Three-dimensional Radiative Heat Transfer in Glass Cooling Processes

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

5. A. Klar, R. Wegener

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

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

Part II: Numerical and stochastic investigations

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

6. A. Klar, N. Siedow

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

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

7. I. Choquet

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

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

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

olution type. Up to now, the homogenization theory has not covered viscoelasticity of the integral type. SanchezPalencia (1980), Francfort & Suquet (1987) (see [2], [9]) have considered homogenization for viscoelasticity of the differential form and only up to the first derivative order. The integral modeled viscoelasticity is more general than the differential one and includes almost all known differential models. The homogenization procedure is based on the construction of an asymptotic solution with respect to a period of the composite structure. This reduces the original problem to some auxiliary boundary value problems of elasticity and viscoelasticity on the unit periodic cell, of the same type as the original non-homogeneous problem. The existence and uniqueness results for such problems were obtained for kernels satisfying some constraint conditions. This is done by the extension of the Volterra integral operator theory to the Volterra operators with respect to the time, whose 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 Wickseil's Corpuscle Problem

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

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

Solving nonconvex planar location problems by finite dominating sets

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

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

Next, it is shown that the approximation of general gauges by polyhedral ones in the objective function of our general model can be analyzed with regard to the subsequent error in the optimal objective value. For the approximation problem two different approaches are described, the sandwich procedure and the greedy algorithm. Both of these approaches lead - for fixed epsilon - to polynomial approximation algorithms with accuracy epsilon for solving the general model considered in this paper.

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

19. A. Becker

A Review on Image Distortion Measures

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

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

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

Polyhedral Properties of the Uncapacitated Multiple Allocation Hub Location Problem

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

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

21. H. W. Hamacher, A. Schöbel

Design of Zone Tariff Systems in Public Transportation

Given a public transportation system represented by its stops and direct connections between stops, we consider two problems dealing with the prices for the customers: The fare problem in which subsets of stops are already aggregated to zones and "good" tariffs have to be found in the existing zone system. Closed form solutions for the fare problem are presented for three objective functions. In the zone problem the design of the zones is part of the problem. This problem is NP

hard and we therefore propose three heuristics which prove to be very successful in the redesign of one of Germany's transportation systems.
(30 pages, 2001)

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

The Finite-Volume-Particle Method for Conservation Laws

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

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

Location Software and Interface with GIS and Supply Chain Management

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

Keywords: facility location, software development,

geographical information systems, supply chain management.

(48 pages, 2001)

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

Mathematical Modelling of Evacuation Problems: A State of Art

This paper details models and algorithms which can be applied to evacuation problems. While it concentrates on building evacuation many of the results are applicable also to regional evacuation. All models consider the time as main parameter, where the travel time between components of the building is part of the input and the overall evacuation time is the output. The paper distinguishes between macroscopic and microscopic evacuation models both of which are able to capture the evacuees' movement over time.

Macroscopic models are mainly used to produce good lower bounds for the evacuation time and do not consider any individual behavior during the emergency situation. These bounds can be used to analyze existing buildings or help in the design phase of planning a building. Macroscopic approaches which are based on dynamic network flow models (minimum cost dynamic flow, maximum dynamic flow, universal maximum flow, quickest path and quickest flow) are described. A special feature of the presented approach is the fact, that travel times of evacuees are not restricted to be constant, but may be density dependent. Using multi-criteria optimization priority regions and blockage due to fire or smoke may be considered. It is shown how the modelling can be done using time parameter either as discrete or continuous parameter.

Microscopic models are able to model the individual evacuee's characteristics and the interaction among evacuees which influence their movement. Due to the corresponding huge amount of data one uses simulation approaches. Some probabilistic laws for individual evacuee's movement are presented. Moreover ideas to model the evacuee's movement using cellular automata (CA) and resulting software are presented. In this paper we will focus on macroscopic models and only summarize some of the results of the microscopic approach. While most of the results are applicable to general evacuation situations, we concentrate on building evacuation.
(44 pages, 2001)

25. J. Kuhnert, S. Tiwari

Grid free method for solving the Poisson equation

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

Keywords: Poisson equation, Least squares method, Grid free method
(19 pages, 2001)

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

Simulation of the fiber spinning process

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

Keywords: Melt spinning, fiber model, Lattice Boltzmann, CFD
(19 pages, 2001)

27. A. Zemitis

On interaction of a liquid film with an obstacle

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

Keywords: impinging jets, liquid film, models, numerical solution, shape
(22 pages, 2001)

28. I. Ginzburg, K. Steiner

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

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

29. H. Neunzert

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

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

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

Keywords: Lehre, Forschung, angewandte Mathematik, Mehrskalanalyse, Strömungsmechanik
(18 pages, 2001)

30. J. Kuhnert, S. Tiwari

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

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

Keywords: Incompressible Navier-Stokes equations, Meshfree method, Projection method, Particle scheme, Least squares approximation
AMS subject classification: 76D05, 76M28
(25 pages, 2001)

31. R. Korn, M. Krekel

Optimal Portfolios with Fixed Consumption or Income Streams

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

Keywords: Portfolio optimisation, stochastic control, HJB equation, discretisation of control problems.
(23 pages, 2002)

32. M. Krekel

Optimal portfolios with a loan dependent credit spread

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

Keywords: Portfolio optimisation, stochastic control, HJB equation, credit spread, log utility, power utility, non-linear wealth dynamics
(25 pages, 2002)

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

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

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

Keywords: image analysis, Euler number, neighborhood relationships, cuboidal lattice
(32 pages, 2002)

34. I. Ginzburg, K. Steiner

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

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

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

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

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

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

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

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

36. S. Feldmann, P. Lang, D. Prätzel-Wolters
Parameter influence on the zeros of network determinants

To a network $N(q)$ with determinant $D(s; q)$ depending on a parameter vector $q \in \mathbb{R}^r$ via identification of some of its vertices, a network $N^\wedge(q)$ is assigned. The paper deals with procedures to find $N^\wedge(q)$, such that its determinant $D^\wedge(s; q)$ admits a factorization in the determinants of appropriate subnetworks, and with the estimation of the deviation of the zeros of D^\wedge from the zeros of D . To solve the estimation problem state space methods are applied.

Keywords: Networks, Equicofactor matrix polynomials, Realization theory, Matrix perturbation theory
(30 pages, 2002)

37. K. Koch, J. Ohser, K. Schladitz
Spectral theory for random closed sets and estimating the covariance via frequency space

A spectral theory for stationary random closed sets is developed and provided with a sound mathematical basis. Definition and proof of existence of the Bartlett spectrum of a stationary random closed set as well as the proof of a Wiener-Khinchine theorem for the power spectrum are used to two ends: First, well known second order characteristics like the covariance

can be estimated faster than usual via frequency space. Second, the Bartlett spectrum and the power spectrum can be used as second order characteristics in frequency space. Examples show, that in some cases information about the random closed set is easier to obtain from these characteristics in frequency space than from their real world counterparts.

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

38. D. d'Humières, I. Ginzburg

Multi-reflection boundary conditions for lattice Boltzmann models

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

Numerical comparisons are given for Stokes flows in periodic arrays of spheres and cylinders, linear periodic array of cylinders between moving plates and for Navier-Stokes flows in periodic arrays of cylinders for $Re < 200$. These results show a significant improvement of the overall accuracy when using the linear interpolations instead of the bounce-back reflection (up to an order of magnitude on the hydrodynamics fields). Further improvement is achieved with the new multi-reflection boundary conditions, reaching a level of accuracy close to the quasi-analytical reference solutions, even for rather modest grid resolutions and few points in the narrowest channels. More important, the pressure and velocity fields in the vicinity of the obstacles are much smoother with multi-reflection than with the other boundary conditions.

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

Keywords: lattice Boltzmann equation, boundary conditions, bounce-back rule, Navier-Stokes equation
(72 pages, 2002)

39. R. Korn

Elementare Finanzmathematik

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

Keywords: Finanzmathematik, Aktien, Optionen, Portfolio-Optimierung, Börse, Lehrerweiterbildung, Mathematikunterricht
(98 pages, 2002)

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

Batch Presorting Problems: Models and Complexity Results

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

Keywords: Complexity theory, Integer programming, Assignment, Logistics
(19 pages, 2002)

41. J. Linn

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

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

Key words: fiber orientation, Folgar-Tucker equation, injection molding
(5 pages, 2003)

42. T. Hanne, S. Nickel

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

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

Key words: multiple objective programming, project management and scheduling, software development, evolutionary algorithms, efficient set
(29 pages, 2003)

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

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

Radiation therapy planning is always a tight rope walk between dangerous insufficient dose in the target volume and life threatening overdosing of organs at risk. Finding ideal balances between these inherently contradictory goals challenges dosimetrists and physicians in their daily practice. Today's planning systems are typically based on a single evaluation function that measures the quality of a radiation treatment plan. Unfortunately, such a one dimensional approach can-

not satisfactorily map the different backgrounds of physicians and the patient dependent necessities. So, too often a time consuming iteration process between evaluation of dose distribution and redefinition of the evaluation function is needed.

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

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

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

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

(31 pages, 2003)

44. T. Halfmann, T. Wichmann

Overview of Symbolic Methods in Industrial Analog Circuit Design

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

Keywords: CAD, automated analog circuit design, symbolic analysis, computer algebra, behavioral modeling, system simulation, circuit sizing, macro modeling, differential-algebraic equations, index

(17 pages, 2003)

45. S. E. Mikhailov, J. Orlik

Asymptotic Homogenisation in Strength and Fatigue Durability Analysis of Composites

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

accumulation rule is employed in the phenomenological micro-durability conditions (for each component of the composite) under varying cyclic loading. Both local and non-local strength and durability conditions are analysed. The strong convergence of the strength and fatigue damage measure as the structure period tends to zero is proved and their limiting values are estimated.

Keywords: multiscale structures, asymptotic homogenization, strength, fatigue, singularity, non-local conditions

(14 pages, 2003)

46. P. Domínguez-Marín, P. Hansen, N. Mladenović, S. Nickel

Heuristic Procedures for Solving the Discrete Ordered Median Problem

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

Keywords: genetic algorithms, variable neighborhood search, discrete facility location

(31 pages, 2003)

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

Exact Procedures for Solving the Discrete Ordered Median Problem

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

Keywords: discrete location, Integer programming

(41 pages, 2003)

48. S. Feldmann, P. Lang

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

A new stability preserving model reduction algorithm for discrete linear SISO-systems based on their impulse response is proposed. Similar to the Padé approximation, an equation system for the Markov parameters involving the Hankel matrix is considered, that here however is chosen to be of very high dimension. Although this equation system therefore in general cannot be solved exactly, it is proved that the approxi-

mate solution, computed via the Moore-Penrose inverse, gives rise to a stability preserving reduction scheme, a property that cannot be guaranteed for the Padé approach. Furthermore, the proposed algorithm is compared to another stability preserving reduction approach, namely the balanced truncation method, showing comparable performance of the reduced systems. The balanced truncation method however starts from a state space description of the systems and in general is expected to be more computational demanding.

Keywords: Discrete linear systems, model reduction, stability, Hankel matrix, Stein equation

(16 pages, 2003)

49. J. Kallrath, S. Nickel

A Polynomial Case of the Batch Presorting Problem

This paper presents new theoretical results for a special case of the batch presorting problem (BPSP). We will show that this case can be solved in polynomial time. Offline and online algorithms are presented for solving the BPSP. Competitive analysis is used for comparing the algorithms.

Keywords: batch presorting problem, online optimization, competitive analysis, polynomial algorithms, logistics

(17 pages, 2003)

50. T. Hanne, H. L. Trinkaus

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

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

Key words: Multicriteria decision making, knowledge management, decision support systems, visual interfaces, interactive navigation, real-life applications.

(26 pages, 2003)

51. O. Iliev, V. Laptev

On Numerical Simulation of Flow Through Oil Filters

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

algorithm. Finally, we present results from simulation of 3-D oil flow through a real car filter.

Keywords: oil filters, coupled flow in plain and porous media, Navier-Stokes, Brinkman, numerical simulation (8 pages, 2003)

52. W. Dörfler, O. Iliev, D. Stoyanov, D. Vassileva
On a Multigrid Adaptive Refinement Solver for Saturated Non-Newtonian Flow in Porous Media

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

Keywords: Nonlinear multigrid, adaptive refinement, non-Newtonian flow in porous media (17 pages, 2003)

53. S. Kruse
On the Pricing of Forward Starting Options under Stochastic Volatility

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

Keywords: Option pricing, forward starting options, Heston model, stochastic volatility, cliquet options (11 pages, 2003)

54. O. Iliev, D. Stoyanov
Multigrid – adaptive local refinement solver for incompressible flows

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

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

55. V. Starikovicius
The multiphase flow and heat transfer in porous media

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

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

56. P. Lang, A. Sarishvili, A. Wirsén
Blocked neural networks for knowledge extraction in the software development process

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

Keywords: Blocked Neural Networks, Nonlinear Regression, Knowledge Extraction, Code Inspection (21 pages, 2003)

57. H. Knaf, P. Lang, S. Zeiser
Diagnosis aiding in Regulation Thermography using Fuzzy Logic

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

Keywords: fuzzy logic, knowledge representation, expert system (22 pages, 2003)

58. M.T. Melo, S. Nickel, F. Saldanha da Gama
Largescale models for dynamic multi-commodity capacitated facility location

In this paper we focus on the strategic design of supply chain networks. We propose a mathematical modeling framework that captures many practical aspects of network design problems simultaneously but which have not received adequate attention in the literature. The aspects considered include: dynamic planning horizon, generic supply chain network structure, external supply of materials, inventory opportunities for goods, distribution of commodities, facility configuration, availability of capital for investments, and storage limitations. Moreover, network configuration decisions concerning the gradual relocation of facilities over the planning horizon are considered. To cope with fluctuating demands, capacity expansion and reduction scenarios are also analyzed as well as modular capacity shifts.

The relation of the proposed modeling framework with existing models is discussed. For problems of reasonable size we report on our computational experience with standard mathematical programming software. In particular, useful insights on the impact of various factors on network design decisions are provided.

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

59. J. Orlik
Homogenization for contact problems with periodically rough surfaces

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

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

60. A. Scherrer, K.-H. Küfer, M. Monz, F. Alonso, T. Bortfeld
IMRT planning on adaptive volume structures – a significant advance of computational complexity

In intensity-modulated radiotherapy (IMRT) planning the oncologist faces the challenging task of finding a treatment plan that he considers to be an ideal compromise of the inherently contradictory goals of delivering a sufficiently high dose to the target while widely sparing critical structures. The search for this a priori unknown compromise typically requires the computation of several plans, i.e. the solution of several optimization problems. This accumulates to a high computa-

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

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

61. D. Kehrwald

Parallel lattice Boltzmann simulation of complex flows

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

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

Status quo: April 2004