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# Vorwort

Das Tätigkeitsfeld des Fraunhofer Instituts für Techno- und Wirtschaftsmathematik ITWM umfasst anwendungsnahe Grundlagenforschung, angewandte Forschung sowie Beratung und kundenspezifische Lösungen auf allen Gebieten, die für Techno- und Wirtschaftsmathematik bedeutsam sind.

In der Reihe »Berichte des Fraunhofer ITWM« soll die Arbeit des Instituts kontinuierlich einer interessierten Öffentlichkeit in Industrie, Wirtschaft und Wissenschaft vorgestellt werden. Durch die enge Verzahnung mit dem Fachbereich Mathematik der Universität Kaiserslautern sowie durch zahlreiche Kooperationen mit internationalen Institutionen und Hochschulen in den Bereichen Ausbildung und Forschung ist ein großes Potenzial für Forschungsberichte vorhanden. In die Berichtreihe sollen sowohl hervorragende Diplom- und Projektarbeiten und Dissertationen als auch Forschungsberichte der Institutsmitarbeiter und Institutsgäste zu aktuellen Fragen der Techno- und Wirtschaftsmathematik aufgenommen werden.

Darüberhinaus bietet die Reihe ein Forum für die Berichterstattung über die zahlreichen Kooperationsprojekte des Instituts mit Partnern aus Industrie und Wirtschaft.

Berichterstattung heißt hier Dokumentation darüber, wie aktuelle Ergebnisse aus mathematischer Forschungs- und Entwicklungsarbeit in industrielle Anwendungen und Softwareprodukte transferiert werden, und wie umgekehrt Probleme der Praxis neue interessante mathematische Fragestellungen generieren.

Prof. Dr. Dieter Prätzel-Wolters
Institutsleiter

Kaiserslautern, im Juni 2001

European Congress on Computational Methods in Applied Sciences and Engineering
ECCOMAS 2004
P. Neittaanmäki, T. Rossi, K. Majava, and O. Pironneau (eds.)
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Jyväskylä, 24–28 July 2004

# ON THE PERFORMANCE OF CERTAIN ITERATIVE SOLVERS FOR COUPLED SYSTEMS ARISING IN DISCRETIZATION OF NON-NEWTONIAN FLOW EQUATIONS

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**Key words:** Performance of iterative solvers, Preconditioners, Non-Newtonian flow.

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

## 1 INTRODUCTION

Efficient numerical simulation of non-Newtonian flows is a non-trivial task. While the numerical methods for Newtonian flows are, in general, well studied, this is not the case for the non-Newtonian fluids. Here we discuss numerical solution of a class of flow problems of so called generalized Newtonian fluids. In this case the viscosity $\mu$ depends on the temperature and on the rate of the strain tensor (in certain cases also on the pressure): $\mu = \mu(T, |\dot{\gamma}|, p)$. As a result, the momentum equations are strongly coupled through their viscous terms (recall, that for Newtonian fluids the coupling of momentum equations is only through the convective terms and the pressure). In the Newtonian case, projection methods for decoupling momentum and continuity equations are often used (for details and further references on fractional time step projection methods of Chorin type, or on SIMPLE-type algorithms, see, e.g., [12, 18, 10, 9]). Decoupling methods might be not efficient in the non-Newtonian case when the momentum equations are strongly coupled. An alternative of the segregated (decoupled) solvers are the so called coupled solvers (see, e.g., [18, 7, 8, 16, 2]). In this case momentum and (transformed) continuity equation are solved together. In the current paper we study the performance of certain iterative solvers for solving such coupled systems, arising in discretization of non-Newtonian flow equations.

The remainder of the paper is organized as follows. Next section presents the governing equations. The discretization is discussed in the third section. Iterative methods and preconditioners for solving coupled system of equations are explained in the fourth section. Fifth section is devoted to numerical experiments and their analysis. Finally, conclusions are drawn in the last section.

## 2 GOVERNING EQUATIONS

Consider unsteady non-isothermal Navier-Stokes equations describing weakly compressible flow of a liquid with variable viscosity (e.g., fluids described by cross WLF model).
Momentum equations are written as :

$$\frac{\partial(\rho u_i)}{\partial t} + div(\rho u_i u) = -\frac{\partial p}{\partial x_i} - \frac{2}{3}\frac{\partial}{\partial x_i}(\mu div(u)) + div(2\mu\dot{\gamma}_i) \tag{1}$$

for the velocity vector components, $u_i$, $i = 1, 2, 3$. Here $\rho$ is the density, $\mu$ is the viscosity, and

$$\dot{\gamma} = \frac{1}{2}(\nabla u + (\nabla u)^T). \tag{2}$$

Continuity equation is written as:

$$\frac{\partial \rho}{\partial t} + div(\rho u) = 0 \tag{3}$$

Energy equation, written with respect to enthalpy $h$, is:

$$\frac{\partial(\rho\ h)}{\partial t} + (\vec{u}, \nabla T) = div(\kappa\ \nabla T) + \mu\ \Phi_V + L\ \frac{\partial f_s}{\partial t}. \tag{4}$$

The last two terms account for the dissipative heating and for latent heat of the phase change, respectively.

Equations of state for density and for viscosity have to be added to the above system. The density depends on the pressure and on the temperature:

$$\rho = \rho(p, T). \tag{5}$$

The viscosity depends on the temperature and on the rate of the strain tensor. Accounting for a pressure dependence is also desirable in certain cases.

$$\mu = \mu(T, |\dot{\gamma}|, p). \tag{6}$$

Particular rheology model and pvT model can be selected from the SIGMASOFT© material database (see www.sigmasoft.de).

The unknowns, to be determined from the above system of equations, are temperature, velocity vector, density, pressure and viscosity:

$$T, \vec{u}, \rho, p, \mu.$$

The above system describes, in particular, flow and solidification of liquid polymer. Simulation of polymer moulding and solidification is of special interest for us, and the main aim of our investigations is to accelerate the flow solver in SIGMASOFT©. In fact, a relatively small time step has to be used in simulating polymer solidification due to the existing free boundaries during the filling of the mold and during solidification. The most CPU consuming part of the calculations is the simulation of the flow at each time step. Motivated by this, below we consider the isothermal case which represents the main difficulties to be overcome. Denote by $C_{\vec{u}}$ and $D_{\vec{u}}$ the operators corresponding to the convective and to the viscous terms in the momentum equations. Obviously, $C_{\vec{u}} = C_{\vec{u}}(\vec{u}),\ \ D_{\vec{u}} = D_{\vec{u}}(\mu(T, |\dot{\gamma}|, p))$ . Further, denote by $G$ and $B$ the operators corresponding to the gradient and divergence. In these notations we can write Navier-Stokes equations as follows:

$$\frac{\partial(\rho\vec{u})}{\partial t} + C_{\vec{u}}\ \vec{u} - D_{\vec{u}}\ \vec{u} + G\ p = 0, \tag{7}$$

$$B\ \vec{u} = 0. \tag{8}$$

Note, that the weak compressibility does not play essential role in the liquid polymer flows we consider, therefore we will not pay special attention to it. Although we solve the weakly compressible equations, here we will discuss the incompressible case, what is enough for our purposes. For a more detailed study on the methods for weakly compressible flows (in the case when this is important) we refer, e.g., to [6, 5, 9] and references therein.

## 3 Discretization

Finite volume method on a staggered grid is applied for discretizing in space the above system of equations (see, e.g., [13] or [10]). Particular form of this space discretization is not discussed here, instead we concentrate on discretiaztion in time and later on, on iterative methods for solving the discretized system.

### 3.1 Fractional time step *projection* methods

Let us shortly consider fractional time step methods which suggest solving the momentum equations in two steps. Projection methods (e.g., Chorin type methods, see, e.g., [12] for a detailed discussion) treat pressure explicitely at the first step, what allows to decouple momentum and continuity equations (the last is used for obtaining an equation with respect to the pressure or to the pressure correction). A variant of such a projection method looks as follows:

$$
\begin{aligned}
(\rho\vec{u})^{n+\frac{1}{2}} + \tau\left(C_{\vec{u}}\vec{u}^{n+\frac{1}{2}} - D_{\vec{u}}\ \vec{u}^{n+\frac{1}{2}}\right) &= (\rho\ \vec{u})^{n} - \tau\ G\ p^{n}, \\
(\rho\vec{u})^{n+1} - (\rho\vec{u})^{n+\frac{1}{2}} &= -\tau\left[G\ p^{n+1} - G\ p^{n}\right], \\
B\ (\rho\vec{u})^{n+1} &= 0.
\end{aligned}
$$

Here we use the superscript $^{n}$ to denote the values at the old time level, and $^{n+1}$ to denote the values at the new time level. Notation $\tau$ stands for the time step, $\tau = t^{n+1} - t^{n}$. The discrete operators are denoted by the same notations as the continuous ones. Viscosity in the diffusive terms and velocity in the convective terms are treated explicitely.

The sum of the first and the second equations above gives an discretization of momentum equations. Applying divergence operator (in our case denoted by $B$) to the second equation, and using the third (continuity) equation, we obtain

$$
\tau BG\delta p = -B(\rho\vec{u})^{n+1} + B(\rho\vec{u})^{n+\frac{1}{2}} = B(\rho\vec{u})^{n+\frac{1}{2}},
$$

where $\delta p = p^{n+1} - p^{n}$. The result of the above Chorin type discretization is a Poisson-type equation for the pressure correction, which is decoupled from the momentum equations. There exist extensive mathematical literature, concerning first and second order fractional time step discretization, incremental and non-incremental form of equations, stability, splitting of the boundary conditions, etc. Some recent results, as well as further references, can be found, e.g., in [4, 14, 1]. Note the Newtonian case, the discretized in this way momentum equations are not coupled, and can be solved consecutively. This is not the case for the non-Newtonian fluids. An attempt to discretize explicitly off-diagonal viscous terms will lead to severe restriction on the time step.

### 3.2 Fractional time step *coupled* method

In the coupled methods the pressure is treated implicitly in the momentum equations. Consider such an approach.

$$
\begin{aligned}
(\rho\vec{u})^{n+\frac{1}{2}} &= (\rho\ \vec{u})^n - \tau C_{\vec{u}}\vec{u}^n - \tau\ G\ p^n, \\
(\rho\vec{u})^{n+1} - (\rho\vec{u})^{n+\frac{1}{2}} &= \tau\left[D_{\vec{u}}\vec{u}^{n+1} - G\ p^{n+1} + G\ p^n\right], \\
B\ (\rho\vec{u})^{n+1} &= 0.
\end{aligned}
$$

Again a Poisson type equation for the pressure correction can be obtained from the second and the third equations, but in this case the system remains coupled, i.e. the second and the transformed third equation have to be solved simultaneously. In fact, in this case we decouple only convective and viscous transport, but keep coupled viscous and pressure forces.

An interesting fractional time step discretization is suggested in [19], but it is not discussed here.

### 3.3 Implicit discretization

If an implicit discretization is used instead of the fractional time step approach, we obtain

$$
\begin{aligned}
(\rho\vec{u})^{n+1} + \tau\left(C_{\vec{u}}\vec{u}^{n+1} - D_{\vec{u}}\vec{u}^{n+1}\right) &= (\rho\ \vec{u})^n - \tau\ G\ p^{n+1}, \\
B\ (\rho\vec{u})^{n+1} &= 0.
\end{aligned}
$$

## 4 Iterative methods for the discretized system

In this section we consider the iterative methods for solving the coupled system of discretized equations. Such a system arises after the implicit discretization, or after the fractional time step coupled discretization. With an obvious change of notations we rewrite the large scale system of linear algebraic equations to be solved at each time step $t = t^{n+1}$ as follows:

$$\begin{pmatrix} A & \tau G \\ B & 0 \end{pmatrix} \begin{pmatrix} \vec{u} \\ p \end{pmatrix} = \begin{pmatrix} S_{\vec{u}} \\ 0 \end{pmatrix}. \tag{9}$$

We will use also notations

$$Lv = b$$

with $v = (\vec{u}, p)^t$.

### 4.1 Iterative projection methods

Iterative projection methods like SIMPLE are discussed in this subsection. Good systematization and detailed references for these methods can be found, e.g., in the book of Turek [18]. One way to derive such methods in the pure incompressible case is as following. Solving the first equation gives us

$$\vec{u} = A^{-1} \left( S_u - \tau G p \right). \tag{10}$$

Substituting in the second equation, we obtain

$$\tau B A^{-1} G p = B A^{-1} S_u. \tag{11}$$

Because $A^{-1}$ is a full matrix, direct solving of the above equation is not possible. Instead, an iterative procedure (preconditioned Richardson method) can be written as

$$p^{i+1} = p^i - M^{-1} \left( \tau B A^{-1} G p^i - B A^{-1} S_u \right) \tag{12}$$

This means that at each iteration we solve

$$M \ \delta p = - \left( \tau B A^{-1} G p^i - B A^{-1} S_u \right) \tag{13}$$

The preconditioner should be spectrally close to $\tau B A^{-1} G$, and at the same time easily invertable. The usual choice is

$$M = \tau B D^{-1} G,$$

where $D$ is a diagonal matrix, so that $M$ is identical to discretization of a second order elliptic operator. For example, in SIMPLE the choice is

$$D = diag A. \tag{14}$$

Let us now consider in more details the matrix $A$. It looks as following:

(i) Constant viscosity:

$$A = \begin{pmatrix} A_{11} & 0 & 0 \\ 0 & A_{22} & 0 \\ 0 & 0 & A_{33} \end{pmatrix}.$$

(ii) Variable viscosity:

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix}.$$

The above representation shows that in the case of strong off-diagonal blocks the approximation of $A$ with an a diagonal matrix $D$ should not be good. It should be noted that even in the Newtonian case (block-diagonal matrix $A$) the decoupling approach might not be successful - an example are flow computations on stretched grids (see, e.g., [18]).

### 4.2 Iterative methods for the coupled system

An alternative for the decoupling approach are coupled solvers. There are different coupled solvers. Few of them work with non transformed system (e.g., Vanka approach [18]), others first transform the system and after that solve. In the CFD literature the coupled solvers are often applied as smoothers within nonlinear multigrid flow solvers (see, e.g. [18, 8, 7]). The coupled solvers require much more memory, compared to segregated solvers. Some software developers (e.g. Fluent) provide both types of solvers. In general, coupled solvers have more restricted area of applicability. It should be mentioned that some authors consider coupled solvers having advantages for steady state solutions, and decoupled techniques being preferable for unsteady problems (see, e.g., [18, 15]). However, very few particular cases are completely analyzed and further studies have to be performed in order to confirm or to reject the above statement. Also, there are observations that the coupled solvers are more robust for some flow problems, and less robust for others, but here also additional work is needed in order to study and classify the advantages of the two approaches.

In this paper we discuss coupled solvers based on proper preconditioning the coupled system (9). Detailed discussion and further references concerning coupled solvers can be found, for example, in [16, 2]. The specific of our approach is described below. A right block triangular preconditioner is used in [16] (the statement in that paper is that left, right, or double sided preconditioning are almost identical). The preconditioner they use is in the form

$$M = \begin{pmatrix} A & R \\ 0 & S \end{pmatrix}.$$

so that

$$LM^{-1} = \begin{pmatrix} I & -(R + \tau G)S^{-1} \\ BA^{-1} & -BA^{-1}RS^{-1} \end{pmatrix}.$$

We do not discuss here the specific choice of operators $R$ and $S$, the interested reader will find them in [16].

Several preconditioners for (9) are carefully analyzed in the recent paper [2]. Among them are block Gauss-Seidel preconditioner, a preconditioner based on congruence transformation, a two-sided block incomplete preconditioner, etc. For example, the block Guass-Seidel preconditioner looks as

$$M = \begin{pmatrix} D_1 & 0 \\ B & D_2 \end{pmatrix}.$$

so that

$$M^{-1}L = \begin{pmatrix} D_1^{-1}A & -D_2^{-1}B(D_1^{-1} - I) \\ \tau D_1^{-1}G & -\tau D_2^{-1}BD_1^{-1}G \end{pmatrix}.$$

For the particular choice of operators $D_1$ and $D_2$, and for discussion on some other preconditioners, we refer to [2].

In general (see, e.g., [3]) applying a preconditioned iterative method for solving a system of equations is equivalent to applying a non-preconditioned method for solving the transformed system. The above approaches [16, 2] are also such examples. Instead of using this approach, we use a two stage approach for solving (9). At the first stage we transform the system using a matrix like above mentioned preconditioners. In the second stage, instead of using unpreconditioned iterative method, we use a preconditioned one. Of course, this two-stage procedure can be written and analyzed as an one-stage one. We postpone such an analysis for another paper, here we concentrate on the algorithmical part and on the numerical study of the performance of the preconditioners. So, at the first stage we use the matrix

$$M^{-1} = \begin{pmatrix} D & 0 \\ -BD & I \end{pmatrix}.$$

so that

$$M^{-1}L = \begin{pmatrix} DA & \tau DG \\ B - BDA & -\tau BDG \end{pmatrix}.$$

The aim of this transformation is to obtain "good" blocks at the main diagonal of the transformed system. It is clear, that the choice $D = A^{-1}$ will lead to a block triangular system, but the operator $BDG$ will have a full matrix in this case. So, like in SIMPLE, we select

$$D = (diag\{A\})^{-1}$$

Thus we obtain an transformed system

$$\tilde{L}v = \tilde{b}, \tag{15}$$

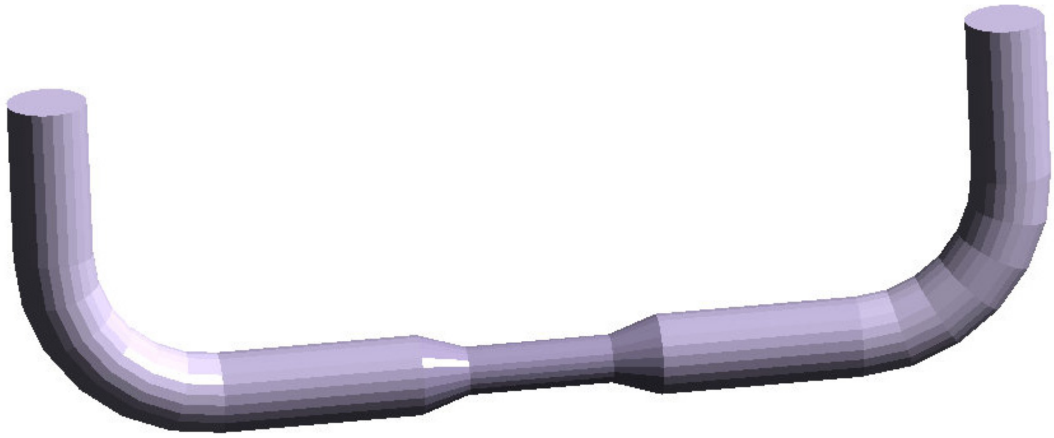

Figure 1: Geometry for evaluating the linear solvers

where $\tilde{L}$ is not a block triangular matrix, however the blocks on the main diagonal are easily invertable (they are similar to a discretization of Poisson equation). This system can be also written down as

$$\begin{pmatrix} \tilde{A} & \tau\tilde{G} \\ \tilde{B} & \tilde{\Lambda} \end{pmatrix} \begin{pmatrix} \vec{u} \\ p \end{pmatrix} = \begin{pmatrix} \tilde{b}_1 \\ b_2 \end{pmatrix}. \quad (16)$$

At the second stage we apply block triangular preconditioners to the transformed system.

## 5 NUMERICAL EXPERIMENTS

Numerical experiments were performed in order to evaluate the performance of the linear solvers applied in the simulation of liquid polymer flow. We choose a simple test geometry shown in Figure 1 consisting of a u-shaped pipe with a contraction and an expansion in the middle. It is well known that the plastic melts do not obey Newtonian behavior, especially near the solidification temperature. A shear thinning behavior is commonly observed for plastic melts. This leads to a necessity of using specific material models for the viscosity including temperature, shear rate and pressure. Several rheology models are available in the material database of SIGMASOFT©, for instance the Cross-WLF model [11]. It belongs to so called generalized Newtonian models, and it is used in our simulations. During the process the viscosity changes by several orders of magnitude.

We solve an unsteady problem, starting simulations from the liquid being in rest, and calculating till the steady state is reached. At each time step the heat equation is decoupled from the system due to an explicit treatment of the dissipative terms and of the velocity in the convective term of the heat equation. The coupled momentum and continuity equations are transformed (as it was described at the end of the preceding section) and after that solved by a preconditioned iterative method. Several methods and preconditioners are applied. More precisely, the used iterative methods are

- CGS: conjugate gradient squared method;
- BiCGStab: bi-conjugate gradient method, stabilized;
- GMRES(m): generalized minimal residuum method

Note, GMRES is the preferred method in [16, 2]. As it will be shown below, in general GMRES is not suitable for us. The simulations show that good convergence can be achieved only using long sequences, what is impossible in 3D simulations due to the memory limitations. Note, that [16, 2] use 'long enough' sequences, but they solve more academic examples.

Concerning the choice of the preconditioners. We have used three preconditioners for the transformed system (16). These are block diagonal, upper triangular (denoted by $T-$ in Tables below), and lower triangular (denoted by $TL-$). That is,

$$\begin{pmatrix} M_{11} & 0 \\ 0 & M_{22} \end{pmatrix}, \qquad T = \begin{pmatrix} M_{11} & M_{12} \\ 0 & M_{22} \end{pmatrix}, \qquad TL = \begin{pmatrix} M_{11} & 0 \\ M_{21} & M_{22} \end{pmatrix}$$

Following variants for the blocks in the preconditioners were used:
- $M_{12} = \tau\tilde{G}$; $M_{21} = \tilde{B}$;
- $M_{11} = ILU_{\tilde{A}}$; $M_{11} = BRILU_{\tilde{A}}$ for various $\alpha$ (calculated for diagonal blocks); $M_{11} = \tilde{A}^{-1}$
- $M_{22} = ILU_{\tilde{\Lambda}}$; $M_{22} = RILU_{\tilde{\Lambda}}$ for various $\alpha$; $M_{22} = \tilde{\Lambda}^{-1}$

In the case when the diagonal blocks have to be inverted, either CGS, Jacobi, GMRES, each preconditioned by RILU($\alpha$) or Block RILU($\alpha$), were used. Additionally, Algebraic multigrid, AMG, [17] was also used for inverting $\tilde{\Lambda}$.

We investigated the performance of the linear solvers with respect to grid size, flow type, accuracy, Re number and the size of the time step. More precisely, the following tests are performed:

| | | |
|---|---|---|
| *Grid:* | coarse, 4584 fluid cells | finer, 38040 fluid cells |
| *flow type:* | Newtonian ( $\mu = const.$) | Non-Newtonian (variable $\mu$) |
| *accuracy:* | lower, $\epsilon = 10^{-3}$ | higher, $\epsilon = 10^{-8}$ |
| *velocity:* | slow, $\Delta p = 10$ | faster, $\Delta p = 30$ |
| *time step:* | smaller | larger |

Table 1: Performed tests for Venturi pipe flow

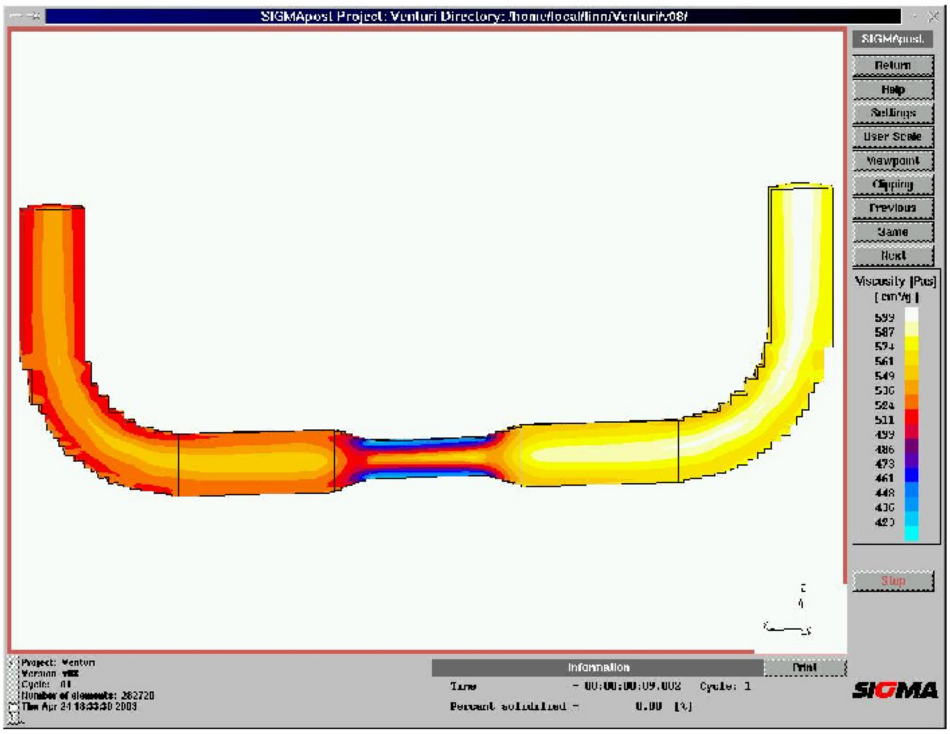


Figure 2: Viscosity

Here $\Delta p$ stands for the pressure difference between the inlet and outlet. The Figure 2 gives an impression about the non-Newtonian case. Variations in the viscosity are plotted there (recall, that viscosity is a constant for Newtonian fluids). Variations in the viscosity here are moderate. In the simulations of solidification of real 3-D plastic parts (results are not shown here, the behavior of the linear solvers is similar) the variation in the viscosity was several orders of magnitude.

Below we show several tables with results from simulations. The block diagonal preconditioner in all cases performed worse compared to the triangular ones, therefore it is not included in the tables.

First, we show four tables presenting results obtained without the usage of AMG. At a last table we show what can be achieved using AMG.

As it can be seen in Table 2, GMRES with short restart sequences does not provide good results. The best results here are achieved by BiCGStab preconditioned with an upper triangular matrix, where the block $M_{11}$ is a block RILU(0.8) factorization for the main sub-blocks of $\tilde{A}$, and $\tilde{\Lambda}$ is approximately inverted by two Jacobi iterations preconditioned with RILU(0.4) factorization. Performing more or less Jacobi iterations gives worser results.

GMRES was not used on the coarse grid (Table 3) because of the bad results it showed on the fine grid. The best iterative method and the best preconditioner on the coarse grid are the same as on the finer grid.

| Preconditioner | CGS | | BiCGStab | | GMRES(10) | |
|---|---|---|---|---|---|---|
| | Iter. | CPU | Iter | CPU | Iter. | CPU |
| T-BILU-ILU | 228 | 31 | 232 | 31 | $> 500$ | |
| T-BRILU0.8-RILU0.4 | 188 | 26 | 149 | 20 | $> 500$ | |
| T-BRILU0.8-*Jac2*RILU0.4 | 138 | 23 | 115 | 18 | $> 500$ | |
| T-*CGS6*BRILU0.8-RILU0.4 | 72 | 282 | 70 | 284 | 122 | 398 |
| TL-BILU-ILU | 224 | 37 | 213 | 34 | $> 500$ | |
| TL-BRILU0.8-RILU0.4 | 180 | 30 | 142 | 23 | $> 500$ | |
| TL-BRILU0.8-*Jac2*RILU0.4 | 138 | 27 | 115 | 22 | $> 500$ | |
| TL-*CGS6*BRILU0.8-RILU0.4 | 60 | 247 | 46 | 195 | 140 | 308 |

Table 2: Number of iteration and CPU time for Non-Newtonian fast flow on fine grid, $\epsilon = 10^{-8}$.

| Preconditioner | CGS | | BiCGStab | | GMRES(10) | |
|---|---|---|---|---|---|---|
| | Iter. | CPU | Iter | CPU | Iter. | CPU |
| T-BILU-ILU | 79 | 1.1 | 67 | 0.9 | | |
| T-BRILU0.8-RILU0.4 | 62 | 0.9 | 58 | 0.8 | | |
| T-BRILU0.8-*Jac2*RILU0.4 | 54 | 0.9 | 47 | 0.7 | | |
| T-*CGS6*BRILU0.8-RILU0.4 | 47 | 7.6 | 46 | 7.4 | | |
| TL-BILU-ILU | 79 | 1.3 | 68 | 1.1 | | |
| TL-BRILU0.8-RILU0.4 | 61 | 1.0 | 56 | 0.9 | | |
| TL-BRILU0.8-*Jac2*RILU0.4 | 52 | 1.0 | 44 | 0.8 | | |
| TL-*CGS6*BRILU0.8-RILU0.4 | 43 | 6.9 | 33 | 5.6 | | |

Table 3: Number of iteration and CPU time for Non-Newtonian fast flow on coarse grid, $\epsilon = 10^{-8}$.

Further, we show results for a non-Newtonian flow with higher variation in the viscosity (Table 4). This is a nonisothermal flow.

Figure 3 shows the behavior of some linear solvers during all the time steps. It can be seen, that the convergence is more or less uniform during the time stepping.

In certain cases there is no need to solve very accurately the linear system arising in discretization of the unsteady PDEs. In Table 5 we show results obtained when low accuracy is required. As it can be seen, in this case the lower triangular preconditioner with an exact inverting of the viscous block shows the best results. This mean that the convergence of the iterative methods is different when using the two different triangular preconditioners. The lower triangular preconditioner ensures fast reduction of the residual at the beginning, but later on the convergence is slower compared to that obtained with the upper triangular preconditioner.

It should be noted that for many industrial problems approximate solution of the linear system of equations is reasonable. In our case the results obtained with $\epsilon = 1e - 3$ and

| Preconditioner | CGS | | BiCGStab | | GMRES | |
|---|---|---|---|---|---|---|
| | Iter. | CPU | Iter | CPU | Iter. | CPU |
| T-BILU-ILU | 185 | 25.2 | 140 | 18.4 | 1063 | 90.4 |
| T-BRILU0.8-RILU0.4 | 129 | 17.6 | 113 | 14.8 | 889 | 75.6 |
| T-BRILU0.8-*Jac2*RILU0.4 | 124 | 20.4 | 116 | 18.4 | 2628 | 263.9 |
| T-*CGS6*BRILU0.8-RILU0.4 | 90 | 262.5 | 83 | 239.7 | 133 | 220.2 |
| TL-BILU-ILU | 172 | 28.3 | 150 | 23.8 | 393 | 88.6 |
| TL-BRILU0.8-RILU0.4 | 135 | 22.1 | 114 | 18.0 | 209 | 46.2 |
| TL-BRILU0.8-*Jac2*RILU0.4 | 125 | 24.0 | 132 | 24.6 | 186 | 43.5 |
| TL-*CGS6*BRILU0.8-RILU0.4 | 52 | 162.2 | 42 | 125.4 | 73 | 125.6 |

Table 4: Number of iteration and CPU time for nonisothermal Non-Newtonian fast flow on coarse grid, $\epsilon = 10^{-8}$.

$\epsilon = 1e - 8$ in many cases show less than 10 pro cent difference.

| Preconditioner | CGS | | BiCGStab | | GMRES | |
|---|---|---|---|---|---|---|
| | Iter. | CPU | Iter | CPU | Iter. | CPU |
| T-BILU-ILU | 45 | 6.2 | 16 | 2.0 | 60 | 5.1 |
| T-BRILU0.8-RILU0.4 | 17 | 2.3 | 16 | 2.0 | 36 | 3.1 |
| T-BRILU0.8-*Jac2*RILU0.4 | 28 | 4.6 | 15 | 2.4 | 121 | 12.3 |
| T-*CGS6*BRILU0.8-RILU0.4 | 18 | 51.8 | 12 | 32.1 | 29 | 44.6 |
| TL-BILU-ILU | 43 | 7.1 | 27 | 4.2 | 56 | 9.3 |
| TL-BRILU0.8-RILU0.4 | 16 | 2.7 | 14 | 2.2 | 41 | 5.9 |
| TL-BRILU0.8-*Jac2*RILU0.4 | 49 | 9.4 | 29 | 5.4 | 43 | 6.9 |
| TL-*CGS6*BRILU0.8-RILU0.4 | 1 | 2.7 | 1 | 1.4 | 1 | 4.0 |

Table 5: Number of iteration and CPU time for nonisothermal Non-Newtonian fast flow on coarse grid, $\epsilon = 10^{-3}$.

Finally, we show some results obtained using algebraic multigrid for inverting $\tilde{\Lambda}$. It can be seen that the results with AMG are superior to other results.

The results obtained with test geometry have been confirmed with several industrial plastic parts. The speedup of the combination of RILU and AMG preconditioner lead to a speedup up to factor 4 for complicated geometries with more than 100.000 fluid cells.

## 6 SUMMARY

The performance of different preconditioners and iterative methods was studied for Venturi geometry, for fast and slow, Newtonian and Non-Newtonian flow, on coarse and on finer grid, for $\epsilon = 10^{-3}$ and $\epsilon = 10^{-8}$, using different time steps.

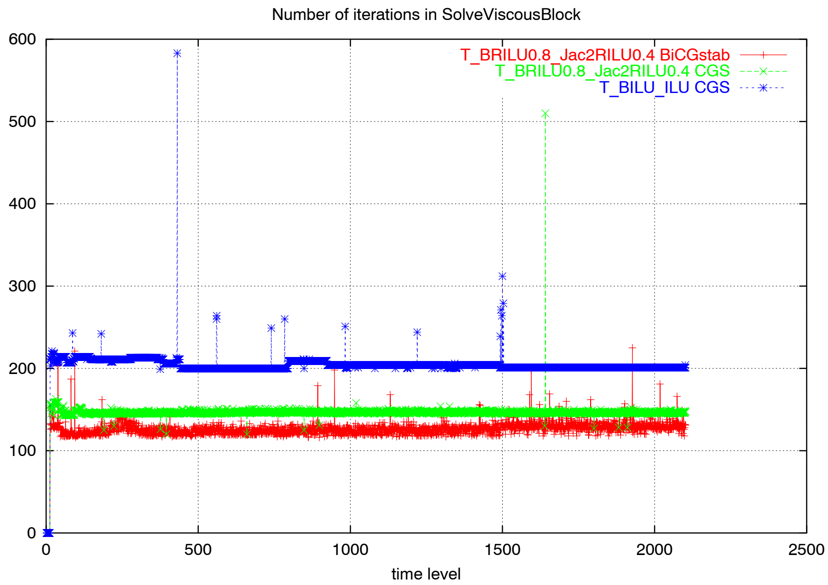


Figure 3: Number of iterations at each time step

The results for Newtonian and Non-Newtonian flows are very close in our calculations. A reason for this might be that we always treat the viscous block (momentum equations) in a coupled way. A more detailed comparison with full segregated solution is in progress now and will be a subject of another paper. Another reason might be the relatively small time step used in our calculations.

We have simulated relatively slow flows, and we did not observe significant differences between our slower and faster regimes. The choice of the velocities in our case was motivated by some practical applications (packing phase of injection molding), for other applications the behavior of the solvers might be different.

BiCGStab has shown the most robust behavior, it was fastest in our tests. GMRES needs long sequences (e.g., 100) for a good convergence, and this is inappropriate for 3-D industrial applications.

Lower triangular preconditioner with inverting the viscous block was the best choice for lower accuracy ($\epsilon = 10^{-3}, \epsilon = 10^{-4}$).

Upper triangular preconditioner, with inverting the Laplacian by Algebraic Multigrid solver was the best choice for high accuracy ($\epsilon = 10^{-8}$).

The presented here results concern the performance of the linear solvers for a particular finite volume discretization and for a particular class of flows. Further studies are planned to better understand the performance of the solvers for other geometries, other non-Newtonian flows and other discretizations.

*Acknowledgments.* This work is partially supported by HYKE: a Research Training Network (RTN) on 'HYperbolic and Kinetic Equations : Asymptotics, Numerics, Analysis', financed by the European Union in the 5th Framework Programme "Improving the

| $\tilde{A}$ Preconditioner | $\tilde{Lambda}$ Preconditioner | Iterative Method | Iterations | Time [s] |
|---|---|---|---|---|
| ILU | ILU | CGS | 182 | 25.6 |
| ILU | ILU | BiCGstab | 194 | 26.3 |
| RILU 0.8 | RILU 0.4 | CGS | 124 | 17.5 |
| RILU 0.8 | RILU 0.4 | BiCGstab | 103 | 14.0 |
| RILU 0.8 | Jac 2 RILU 0.4 | CGS | 105 | 17.7 |
| RILU 0.8 | Jac 2 RILU 0.4 | BiCGstab | 84 | 13.7 |
| CGS 6 RILU 0.8 | RILU 0.4 | CGS | 82 | 172.5 |
| CGS 6 RILU 0.8 | RILU 0.4 | BiCGstab | 68 | 144.8 |
| RILU 0.8 | AMG V | CGS | 44 | $\approx$ 6.9 |
| RILU 0.8 | AMG V | BiCGstab | 41 | $\approx$ 5.0 |

Table 6: Number of iteration and CPU time for nonisothermal Non-Newtonian flow on fine grid, $\epsilon = 10^{-8}$.

Human Potential" (IHP). Project Reference : Contract Number : HPRN-CT-2002-00282.

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# Published reports of the Fraunhofer ITWM

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

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

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

6. A. Klar, N. Siedow
***Boundary Layers and Domain Decomposition for Radiative Heat Transfer and Diffusion Equations: Applications to Glass Manufacturing Processes***
In this paper domain decomposition methods for radiative transfer problems including conductive heat transfer are treated. The paper focuses on semi-transparent materials, like glass, and the associated conditions at the interface between the materials. Using asymptotic analysis we derive conditions for the coupling of the radiative transfer equations and a diffusion approximation. Several test cases are treated and a problem appearing in glass manufacturing processes is computed. The results clearly show the advantages of a domain decomposition approach. Accuracy equivalent to the solution of the global radiative transfer solution is achieved, whereas computation time is strongly reduced.
(24 pages, 1998)

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

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

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

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

10. J. Mohring

**_Helmholtz Resonators with Large Aperture_**

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

11. H. W. Hamacher, A. Schöbel

**_On Center Cycles in Grid Graphs_**

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

12. H. W. Hamacher, K.-H. Küfer

**_Inverse radiation therapy planning - a multiple objective optimisation approach_**

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

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

**_On the Analysis of Spatial Binary Images_**

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

14. M. Junk

**_On the Construction of Discrete Equilibrium Distributions for Kinetic Schemes_**

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

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

**_A new discrete velocity method for Navier-Stokes equations_**

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

16. H. Neunzert

**_Mathematics as a Key to Key Technologies_**

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

17. J. Ohser, K. Sandau

**_Considerations about the Estimation of the Size Distribution in Wicksell’s Corpuscle Problem_**

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

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

**_Solving nonconvex planar location problems by finite dominating sets_**

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

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

19. A. Becker

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

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

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

**Polyhedral Properties of the Uncapacitat*ed Multiple Allocation Hub Location Problem***

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

21. H. W. Hamacher, A. Schöbel

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

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

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

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

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

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

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

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

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

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

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

25. J. Kuhnert, S. Tiwari

***Grid free method for solving the Poisson equation***

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

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

***Simulation of the fiber spinning process***

To simulate the influence of process parameters to the melt spinning process a fiber model is used and coupled with CFD calculations of the quench air flow. In the fiber model energy, momentum and mass balance are solved for the polymer mass flow. To calculate the quench air the Lattice Boltzmann method is used. Simulations and experiments for different process parameters and hole configurations are compared and show a good agreement.
*Keywords: Melt spinning, fiber model, Lattice Boltzmann, CFD*
(19 pages, 2001)

27. A. Zemitis

***On interaction of a liquid film with an obstacle***

In this paper mathematical models for liquid films generated by impinging jets are discussed. Attention is stressed to the interaction of the liquid film with some obstacle. S. G. Taylor [Proc. R. Soc. London Ser. A 253, 313 (1959)] found that the liquid film generated by impinging jets is very sensitive to properties of the wire which was used as an obstacle. The aim of this presentation is to propose a modification of the Taylor's model, which allows to simulate the film shape in cases, when the angle between jets is different from 180°. Numerical results obtained by discussed models give two different shapes of the liquid film similar as in Taylors experiments. These two shapes depend on the regime: either droplets are produced close to the obstacle or not. The difference between two regimes becomes larger if the angle between jets decreases. Existence of such two regimes can be very essential for some applications of impinging jets, if the generated liquid film can have a contact with obstacles.
*Keywords: impinging jets, liquid film, models, numerical solution, shape*
(22 pages, 2001)

28. I. Ginzburg, K. Steiner

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

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

29. H. Neunzert

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

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

Was macht einen guten Hochschullehrer aus? Auf diese Frage gibt es sicher viele verschiedene, fachbezogene Antworten, aber auch ein paar allgemeine Gesichtspunkte: es bedarf der »Leidenschaft« für die Forschung (Max Weber), aus der dann auch die Begeisterung für die Lehre erwächst. Forschung und Lehre gehören zusammen, um die Wissenschaft als lebendiges Tun vermitteln zu können. Der Vortrag gibt Beispiele dafür, wie in angewandter Mathematik Forschungsaufgaben aus praktischen Alltagsproblemstellungen erwachsen, die in die Lehre auf verschiedenen Stufen (Gymnasium bis Graduiertenkolleg) einfließen; er leitet damit auch zu einem aktuellen Forschungsgebiet, der Mehrskalenanalyse mit ihren vielfältigen Anwendungen in Bildverarbeitung, Materialentwicklung und Strömungsmechanik über, was aber nur kurz gestreift wird. Mathematik erscheint hier als eine moderne Schlüsseltechnologie, die aber auch enge Beziehungen zu den Geistes- und Sozialwissenschaften hat.
*Keywords: Lehre, Forschung, angewandte Mathematik, Mehrskalenanalyse, Strömungsmechanik*
(18 pages, 2001)

30. J. Kuhnert, S. Tiwari

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

A Lagrangian particle scheme is applied to the projection method for the incompressible Navier-Stokes equations. The approximation of spatial derivatives is obtained by the weighted least squares method. The pressure Poisson equation is solved by a local iterative procedure with the help of the least squares method. Numerical tests are performed for two dimensional cases. The Couette flow, Poiseuelle flow, decaying shear flow and the driven cavity flow are presented. The numerical solutions are obtained for stationary as well as instationary cases and are compared with the analytical solutions for channel flows. Finally, the driven cavity in a unit square is considered and the stationary solution obtained from this scheme is compared with that from the finite element method.
*Keywords: Incompressible Navier-Stokes equations, Meshfree method, Projection method, Particle scheme, Least squares approximation*
*AMS subject classification: 76D05, 76M28*
(25 pages, 2001)

31. R. Korn, M. Krekel

***Optimal Portfolios with Fixed Consumption or Income Streams***

We consider some portfolio optimisation problems where either the investor has a desire for an a priori specified consumption stream or/and follows a deterministic pay in scheme while also trying to maximize expected utility from final wealth. We derive explicit closed form solutions for continuous and discrete monetary streams. The mathematical method used is classical stochastic control theory.
*Keywords: Portfolio optimisation, stochastic control, HJB equation, discretisation of control problems.*
(23 pages, 2002)

32. M. Krekel

***Optimal portfolios with a loan dependent credit spread***

If an investor borrows money he generally has to pay higher interest rates than he would have received, if he had put his funds on a savings account. The classical model of continuous time portfolio optimisation ignores this effect. Since there is obviously a connection between the default probability and the total percentage of wealth, which the investor is in debt, we study portfolio optimisation with a control dependent interest rate. Assuming a logarithmic and a power utility function, respectively, we prove explicit formulae of the optimal control.
*Keywords: Portfolio optimisation, stochastic control, HJB equation, credit spread, log utility, power utility, non-linear wealth dynamics*
(25 pages, 2002)

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

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

Two approaches for determining the Euler-Poincaré characteristic of a set observed on lattice points are considered in the context of image analysis { the integral geometric and the polyhedral approach. Information about the set is assumed to be available on lattice points only. In order to retain properties of the Euler number and to provide a good approximation of the true Euler number of the original set in the Euclidean space, the appropriate choice of adjacency in the lattice for the set and its background is crucial. Adjacencies are defined using tessellations of the whole space into polyhedrons. In R 3 , two new 14 adjacencies are introduced additionally to the well known 6 and 26 adjacencies. For the Euler number of a set and its complement, a consistency relation holds. Each of the pairs of adjacencies (14:1; 14:1), (14:2; 14:2), (6; 26), and (26; 6) is shown to be a pair of complementary adjacencies with respect to this relation. That is, the approximations of the Euler numbers are consistent if the set and its background (complement) are equipped with this pair of adjacencies. Furthermore, sufficient conditions for the correctness of the approximations of the Euler number are given. The analysis of selected microstructures and a simulation study illustrate how the estimated Euler number depends on the chosen adjacency. It also shows that there is not a uniquely best pair of adjacencies with respect to the estimation of the Euler number of a set in Euclidean space.
*Keywords: image analysis, Euler number, neighborhod relationships, cuboidal lattice*
(32 pages, 2002)

34. I. Ginzburg, K. Steiner

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

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

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

35. M. Günther, A. Klar, T. Materne, R. Wegener
***Multivalued fundamental diagrams and stop and go waves for continuum traffic equations***

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

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

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

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

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

38. D. d'Humières, I. Ginzburg
***Multi-reflection boundary conditions for lattice Boltzmann models***

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

39. R. Korn
***Elementare Finanzmathematik***

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

40. J. Kallrath, M. C. Müller, S. Nickel
***Batch Presorting Problems: Models and Complexity Results***

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

41. J. Linn
***On the frame-invariant description of the phase space of the Folgar-Tucker equation***

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

42. T. Hanne, S. Nickel
***A Multi-Objective Evolutionary Algorithm for Scheduling and Inspection Planning in Software Development Projects***

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

43. T. Bortfeld , K.-H. Küfer, M. Monz, A. Scherrer, C. Thieke, H. Trinkaus
***Intensity-Modulated Radiotherapy - A Large Scale Multi-Criteria Programming Problem -***

Radiation therapy planning is always a tight rope walk between dangerous insufficient dose in the target volume and life threatening overdosing of organs at risk. Finding ideal balances between these inherently contradictory goals challenges dosimetrists and physicians in their daily practice. Today's planning systems are typically based on a single evaluation function that measures the quality of a radiation treatment plan. Unfortunately, such a one dimensional approach 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 approximate solution, computed via the Moore-Penrose inverse, gives rise to a stability preserving reduction scheme, a property that cannot be guaranteed for the Padé approach. Furthermore, the proposed algorithm is compared to another stability preserving reduction approach, namely the balanced truncation method, showing comparable performance of the reduced systems. The balanced truncation method however starts from a state space description of the systems and in general is expected to be more computational demanding.
*Keywords: Discrete linear systems, model reduction, stability, Hankel matrix, Stein equation*
(16 pages, 2003)

49. J. Kallrath, S. Nickel

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

This paper presents new theoretical results for a special case of the batch presorting problem (BPSP). We will show tht this case can be solved in polynomial time. Offline and online algorithms are presented for solving the BPSP. Competetive analysis is used for comparing the algorithms.
*Keywords: batch presorting problem, online optimization, competetive 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 haycocks", the knowledge navigation component supports graphical database retrieval and interactive, goal-oriented problem solving. Navigation "helpers" are, for instance, cascading criteria aggregations, modifiable metrics, ergonomic interfaces, and customizable visualizations. Examples from real-life projects, e.g. in industrial engineering and in the life sciences, illustrate the application of our MCDSS.
*Key words: Multicriteria decision making, knowledge management, decision support systems, visual interfaces, interactive navigation, real-life applications.*
(26 pages, 2003)

51. O. Iliev, V. Laptev

***On Numerical Simulation of Flow Through Oil Filters***

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

algorithm. Finally, we present results from simulation of 3-D oil flow through a real car filter.
*Keywords: oil filters, coupled flow in plain and porous media, Navier-Stokes, Brinkman, numerical simulation*
(8 pages, 2003)

52. W. Dörfler, O. Iliev, D. Stoyanov, D. Vassileva
***On a Multigrid Adaptive Refinement Solver for Saturated Non-Newtonian Flow in Porous Media***
A multigrid adaptive refinement algorithm for non-Newtonian flow in porous media is presented. The saturated flow of a non-Newtonian fluid is described by the continuity equation and the generalized Darcy law. The resulting second order nonlinear elliptic equation is discretized by a finite volume method on a cell-centered grid. A nonlinear full-multigrid, full-approximation-storage algorithm is implemented. As a smoother, a single grid solver based on Picard linearization and Gauss-Seidel relaxation is used. Further, a local refinement multigrid algorithm on a composite grid is developed. A residual based error indicator is used in the adaptive refinement criterion. A special implementation approach is used, which allows us to perform unstructured local refinement in conjunction with the finite volume discretization. Several results from numerical experiments are presented in order to examine the performance of the solver.
*Keywords: Nonlinear multigrid, adaptive refinement, non-Newtonian flow in porous media*
(17 pages, 2003)

53. S. Kruse
***On the Pricing of Forward Starting Options under Stochastic Volatility***
We consider the problem of pricing European forward starting options in the presence of stochastic volatility. By performing a change of measure using the asset price at the time of strike determination as a numeraire, we derive a closed-form solution based on Heston's model of stochastic volatility.
*Keywords: Option pricing, forward starting options, Heston model, stochastic volatility, cliquet options*
(11 pages, 2003)

54. O. Iliev, D. Stoyanov
***Multigrid – adaptive local refinement solver for incompressible flows***
A non-linear multigrid solver for incompressible Navier-Stokes equations, exploiting finite volume discretization of the equations, is extended by adaptive local refinement. The multigrid is the outer iterative cycle, while the SIMPLE algorithm is used as a smoothing procedure. Error indicators are used to define the refinement subdomain. A special implementation approach is used, which allows to perform unstructured local refinement in conjunction with the finite volume discretization. The multigrid - adaptive local refinement algorithm is tested on 2D Poisson equation and further is applied to a lid-driven flows in a cavity (2D and 3D case), comparing the results with bench-mark data. The software design principles of the solver are also discussed.
*Keywords: Navier-Stokes equations, incompressible flow, projection-type splitting, SIMPLE, multigrid methods, adaptive local refinement, lid-driven flow in a cavity*
(37 pages, 2003)

55. V. Starikovicius
***The multiphase flow and heat transfer in porous media***
In first part of this work, summaries of traditional Multiphase Flow Model and more recent Multiphase Mixture Model are presented. Attention is being paid to attempts include various heterogeneous aspects into models. In second part, MMM based differential model for two-phase immiscible flow in porous media is considered. A numerical scheme based on the sequential solution procedure and control volume based finite difference schemes for the pressure and saturation-conservation equations is developed. A computer simulator is built, which exploits object-oriented programming techniques. Numerical result for several test problems are reported.
*Keywords: Two-phase flow in porous media, various formulations, global pressure, multiphase mixture model, numerical simulation*
(30 pages, 2003)

56. P. Lang, A. Sarishvili, A. Wirsen
***Blocked neural networks for knowledge extraction in the software development process***
One of the main goals of an organization developing software is to increase the quality of the software while at the same time to decrease the costs and the duration of the development process. To achieve this, various decisions e.ecting 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 di.erent objects involved in the development process. Based on experimental data, techniques from the .eld 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 quanti.cation 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 multicommodity 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 micropeaks and valleys is very small compared with the macrosize 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 macrolevel. The averaged contact stiffness obtained allows the replacement of the interface layer in the macromodel by the macrocontact condition.
*Keywords: asymptotic homogenization, contact problems*
(28 pages, 2004)

60. A. Scherrer, K.-H. Küfer, M. Monz, F. Alonso, T. Bortfeld
***IMRT planning on adaptive volume structures – a significant advance of computational complexity***
In intensity-modulated radiotherapy (IMRT) planning the oncologist faces the challenging task of finding a treatment plan that he considers to be an ideal compromise of the inherently contradictive 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)

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

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

Iterative solution of large scale systems arising after discretization and linearization of the unsteady non-Newtonian Navier–Stokes equations is studied. cross WLF model is used to account for the non-Newtonian behavior of the fluid. Finite volume method is used to discretize the governing system of PDEs. Viscosity is treated explicitely (e.g., it is taken from the previous time step), while other terms are treated implicitly. Different preconditioners (block–diagonal, block–triangular, relaxed incomplete LU factorization, etc.) are used in conjunction with advanced iterative methods, namely, BiCGStab, CGS, GMRES. The action of the preconditioner in fact requires inverting different blocks. For this purpose, in addition to preconditioned BiCGStab, CGS, GMRES, we use also algebraic multigrid method (AMG). The performance of the iterative solvers is studied with respect to the number of unknowns, characteristic velocity in the basic flow, time step, deviation from Newtonian behavior, etc. Results from numerical experiments are presented and discussed.
*Keywords: Performance of iterative solvers, Preconditioners, Non-Newtonian flow*
(17 pages, 2004)

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

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

In this paper we consider numerical algorithms for solving a system of nonlinear PDEs arising in modeling of liquid polymer injection. We investigate the particular case when a porous preform is located within the mould, so that the liquid polymer flows through a porous medium during the filling stage. The nonlinearity of the governing system of PDEs is due to the non-Newtonian behavior of the polymer, as well as due to the moving free boundary. The latter is related to the penetration front and a Stefan type problem is formulated to account for it. A finite-volume method is used to approximate the given differential problem. Results of numerical experiments are presented.
We also solve an inverse problem and present algorithms for the determination of the absolute preform permeability coefficient in the case when the velocity of the penetration front is known from measurements. In both cases (direct and inverse problems) we emphasize on the specifics related to the non-Newtonian behavior of the polymer. For completeness, we discuss also the Newtonian case. Results of some experimental measurements are presented and discussed.
*Keywords: Liquid Polymer Moulding, Modelling, Simulation, Infiltration, Front Propagation, non-Newtonian flow in porous media*
(43 pages, 2004)

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