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R. Ciegis, O. Iliev, V. Starikovicius, K. Steiner

## Numerical Algorithms for Solving Problems of Multiphase Flows in Porous Media

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Fraunhofer-Institut für Techno- und  
Wirtschaftsmathematik ITWM  
Fraunhofer-Platz 1

67663 Kaiserslautern  
Germany

Telefon: +49(0)6 31/3 16 00-10 10  
Telefax: +49(0)6 31/3 16 00-10 99  
E-Mail: [info@itwm.fraunhofer.de](mailto:info@itwm.fraunhofer.de)  
Internet: [www.itwm.fraunhofer.de](http://www.itwm.fraunhofer.de)

# 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.

A handwritten signature in black ink, reading "Dieter Prätzel-Wolters". The signature is fluid and cursive, with the first name "Dieter" and last name "Prätzel-Wolters" clearly distinguishable.

Prof. Dr. Dieter Prätzel-Wolters  
Institutsleiter

Kaiserslautern, im Juni 2001



## NUMERICAL ALGORITHMS FOR SOLVING PROBLEMS OF MULTIPHASE FLOWS IN POROUS MEDIA

R. ČIEGIS<sup>1</sup>, O. ILIEV<sup>2</sup>, V. STARIKOVIČIUS<sup>1</sup> and K. STEINER<sup>2</sup>

<sup>1</sup>*Vilnius Gediminas Technical University*

Saulėtekio al. 11, LT-10223, Vilnius, Lithuania

E-mail: rc@fm.vtu.lt

<sup>2</sup>*Fraunhofer ITWM*

Fraunhofer-Platz 1, D-67663 Kaiserslautern, Germany

E-mail: iliev@itwm.fhg.de

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**Abstract.** In this paper we discuss numerical algorithms for solving the system of nonlinear PDEs, arising in modelling of two-phase flows in porous media, as well as the proper object oriented implementation of these algorithms. Global pressure model for isothermal two-phase immiscible flow in porous media is considered in this paper. Finite-volume method is used for the space discretization of the system of PDEs. Different time stepping discretizations and linearization approaches are discussed. The main concepts of the PDE software tool *MfsolverC++* are given. Numerical results for one realistic problem are presented.

**Key words:** nonlinear algorithms, finite-volume method, software tools, porous media, flows

### 1. Introduction

Problems involving the multiphase flow, heat transfer, and multicomponent mass transport in porous media arise in a broad spectrum of engineering disciplines. Important technological applications include the drying of porous solids and soils, subsurface contamination and remediation, thermally enhanced oil recovery, geothermal energy production, porous heat pipes, nuclear reactor safety analysis, high-level secure radioactive waste repositories, paper machines.

Mathematical models for multiphase flow in porous media usually are formulated at macroscopic level and they are obtained by volume averaging or

homogenization methods from microscopic equations. The transport phenomena are mathematically described by the basic principles of conservation for each phase separately and by appropriate interfacial conditions between various phases.

The resulting models are difficult to solve due to large number of strongly coupled nonlinear differential equations in the systems.

In this paper we solve numerically global pressure model for isothermal two-phase immiscible flow problems. The model is described in Section 2. In Section 3 we present the chosen finite volume discretization, and discuss numerical difficulties connected to different approaches for time discretization and for linearization of the governing system of PDEs. Section 4 describes the concept of our software tool for the solution of multiphase flow problems, called `MfsolverC++`, as well as the current state of the implementations. Results of computational experiments are presented in Section 5.

## 2. Global Pressure Model for Isothermal Two-Phase Immiscible Flow in Porous Media

Traditionally multiphase flow in porous media is described by the macroscopic models, in which various phases are considered as distinct fluids with individual thermodynamic and transport properties [6]. Macroscopic equations are obtained by averaging microscopic equations over the representative elementary volume. The microscopic equations are the equations of mass, momentum and energy conservation for all considered phases. The change of scale enables to convert the real discontinuous medium to a fictitious continuous one. Each macroscopic term is obtained by averaging microscopic ones. The averaging (integration) is done by using various closing assumptions (homogeneity, periodic cell structure etc.) [35].

So, for isothermal two-phase immiscible flow in porous media we have 2 equations for mass conservation in each phase ( $k = 1, 2$ ):

$$\varepsilon \frac{\partial (\rho_k s_k)}{\partial t} + \nabla \cdot (\rho_k \mathbf{u}_k) = 0, \quad (2.1)$$

where  $\varepsilon$  is the porosity of the porous medium,  $\rho_k$  is the phase density,  $s_k$  is the phase saturation denoting the volumetric fraction of the void space occupied by phase  $k$ . Obviously we have

$$s_1 + s_2 = 1.$$

$\mathbf{u}_k$  is the macroscopic velocity vector (volume rate of flow through a unit cross-sectional area of multiple fluids and porous medium). It is also called bulk velocity. It is assumed that there are no external mass sources or sinks, no mass transfer between phases, and the porous medium is not deformable.

It is also assumed that multiphase extension of Darcy's law is valid for conservation of phase momentum:

$$\mathbf{u}_k = -\mathbf{K} \frac{k_{rk}}{\mu_k} (\nabla p_k - \rho_k \mathbf{g}), \quad (2.2)$$

where  $\mathbf{K}$  is the absolute permeability tensor of the porous medium,  $k_{rk}$  is the relative permeability of phase  $k$ ,  $\mu_k$  is the phase dynamic viscosity,  $p_k$  is the phase pressure, and  $\mathbf{g}$  is the gravitational vector. The pressures of two phases are related through the capillary pressure,  $p_c = p_2 - p_1$ . Relative permeability functions and capillary pressure are assumed to be functions of the phase saturations only

$$k_{rk} = k_{rk}(s_k), \quad p_c = p_c(s_1). \quad (2.3)$$

One of the assumptions in generalized Darcy's law is that flow is slow, i.e. inertial effects can be neglected.

The governing equations (2.1)–(2.2) can be mathematically manipulated into several alternate forms with different choices of primary variables: saturation–pressure, pressure–pressure, saturation–saturation formulations. We have chosen global pressure model, sometimes also called fractional flow formulation [7] or mixture model. Comparing to other formulations, equations in this model are less coupled and entering quantities are smoother, because most of them describe mixture properties: velocity, density, etc.

First we define the properties of multiphase mixture through the properties of its components (phases). The mixture density and velocity are defined, respectively, as

$$\rho = \rho_1 s_1 + \rho_2 s_2, \quad (2.4)$$

$$\rho \mathbf{u} = \rho_1 \mathbf{u}_1 + \rho_2 \mathbf{u}_2. \quad (2.5)$$

The mixture kinematic viscosity is given by

$$\nu = \left( \frac{k_{r1}}{\nu_1} + \frac{k_{r2}}{\nu_2} \right)^{-1}, \quad (2.6)$$

where  $\nu_k = \mu_k / \rho_k$  is the kinematic viscosity of phase  $k$ . Then, the mobility of each phase in the multiphase mixture is defined as

$$\lambda_k = \frac{k_{rk}}{\nu_k} \nu, \quad (2.7)$$

In the literature,  $\lambda_k$  is often called the fractional flow function. We have the following relation for these functions:

$$\lambda_1 + \lambda_2 = 1.$$

The main idea of the model is an introduction of the global (mixture) pressure. The mixture pressure is defined so that the following differential equation holds:

$$\nabla p = \lambda_1 \nabla p_1 + \lambda_2 \nabla p_2 = \nabla p_1 + \lambda_2 \nabla p_c.$$

It is not always possible to find such  $p$ . A necessary condition for this is the interchangeability of partial derivatives:

$$\frac{\partial}{\partial x_i} \left( \lambda_2 \frac{\partial p_c}{\partial x_j} \right) = \frac{\partial}{\partial x_j} \left( \lambda_2 \frac{\partial p_c}{\partial x_i} \right), \quad i \neq j.$$

For our assumptions this condition is satisfied, and mixture pressure can be defined explicitly as

$$\begin{aligned} p &= p_1 + \int_{S_c}^{s_1} \lambda_2(\xi) \frac{dp_c}{d\xi} d\xi = p_2 - \int_{S_c}^{s_1} \lambda_1(\xi) \frac{dp_c}{d\xi} d\xi \\ &= \frac{p_1 + p_2}{2} + \frac{1}{2} \int_{S_c}^{s_1} (\lambda_2(\xi) - \lambda_1(\xi)) \frac{dp_c}{d\xi} d\xi, \end{aligned} \quad (2.8)$$

where  $S_c$  is obtained from the equation  $p_c(S_c) = 0$ .

Adding the phase mass conservation equations (2.1) we obtain the continuity equation for the mixture:

$$\varepsilon \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0. \quad (2.9)$$

Multiplying equations (2.2) by corresponding densities and summing them up, we obtain Darcy's law for the mixture:

$$\rho \mathbf{u} = -\frac{\mathbf{K}}{\nu} (\nabla p - (\lambda_1 \rho_1 + \lambda_2 \rho_2) \mathbf{g}). \quad (2.10)$$

Substituting (2.10) into (2.9) we get

$$\varepsilon \frac{\partial \rho}{\partial t} - \nabla \cdot \left( \frac{\mathbf{K}}{\nu} (\nabla p - (\lambda_1 \rho_1 + \lambda_2 \rho_2) \mathbf{g}) \right) = 0. \quad (2.11)$$

Obtained equation is sometimes called pressure equation and is used to find global (mixture) pressure  $p$ . The mixture kinematic viscosity  $\nu$  is positive. The absolute permeability tensor  $\mathbf{K}$  of porous medium is positive-definite, so is  $\mathbf{K}/\nu$ . Consequently, it follows from (2.11) that the pressure equation is *elliptic* (for known  $\rho$ ).

The diffusive mass flux of phase  $k$  within the multiphase mixture is defined as

$$\mathbf{j}_k = \rho_k \mathbf{u}_k - \lambda_k \rho \mathbf{u}, \quad (2.12)$$

or alternatively,

$$\rho_k \mathbf{u}_k = \mathbf{j}_k + \lambda_k \rho \mathbf{u}. \quad (2.13)$$

As a consequence we get that

$$\mathbf{j}_1 + \mathbf{j}_2 = 0.$$

Substituting the momentum equations for the first phase (2.2) and for the mixture (2.10) into equation (2.12), the diffusive mass flux  $\mathbf{j}_1$  can be expressed as follows:

$$\mathbf{j}_1 = \frac{\mathbf{K} \lambda_1 \lambda_2}{\nu} (\nabla p_c + (\rho_1 - \rho_2) \mathbf{g}). \quad (2.14)$$



Substituting equations (2.13) with  $k = 1$  and (2.14) into mass conservation equation of the first phase (2.1), we obtain

$$\varepsilon \frac{\partial (\rho_1 s_1)}{\partial t} + \nabla \cdot (\rho \mathbf{u} \lambda_1) = -\nabla \cdot \left( \frac{\mathbf{K} \lambda_1 \lambda_2}{\nu} (\nabla p_c + (\rho_1 - \rho_2) \mathbf{g}) \right). \quad (2.15)$$

Equation (2.15) is called a saturation equation. It is used to find the saturation  $s_1$ . Note that  $dp_c/ds_1 < 0$  by the property of capillary pressure. Hence if  $\mathbf{K}$  is positive-definite, then (2.15) is a degenerate parabolic equation. The degeneracy is caused by the fact that fractional mobilities  $\lambda_1$  and  $\lambda_2$  can become zero. When the capillary forces are small, saturation equation (2.15) is advection dominated. It is purely hyperbolic in the absence of the diffusive forces.

The saturation equation (2.15) in conjunction with the pressure equation (2.11) and the Darcy law (2.10) makes up a full system of equations for unknowns  $p$ ,  $\mathbf{u}$ , and  $s_1$ :

$$\begin{cases} \varepsilon \frac{\partial \rho}{\partial t} - \nabla \cdot \left( \frac{\mathbf{K}}{\nu} (\nabla p - (\lambda_1 \rho_1 + \lambda_2 \rho_2) \mathbf{g}) \right) = 0, \\ \rho \mathbf{u} = -\frac{\mathbf{K}}{\nu} (\nabla p - (\lambda_1 \rho_1 + \lambda_2 \rho_2) \mathbf{g}), \\ \varepsilon \frac{\partial (\rho_1 s_1)}{\partial t} + \nabla \cdot (\rho \mathbf{u} \lambda_1) = -\nabla \cdot \left( \frac{\mathbf{K} \lambda_1 \lambda_2}{\nu} (\nabla p_c + (\rho_1 - \rho_2) \mathbf{g}) \right). \end{cases} \quad (2.16)$$

The system is completed by the constitutive relations (2.3). Equations are defined in  $\Omega$ , which is assumed to be a polyhedral domain. Both, Dirichlet and full flux (or Neumann) type boundary conditions can be specified on the boundary  $\partial\Omega$  of the region.

This system can be used to model isothermal two-phase immiscible fluid flow in porous media, when the phase compositions are of no importance and molecular diffusion and hydraulic dispersion effects can be neglected.

### 3. Numerical Algorithms

The major numerical difficulties for problems arising in the simulation of processes in porous media are identified by Ewing [14] and Helmig [17] (see also the dissertation of Bastian [4]). They deal with

- solution of convection dominated parabolic problems,
- time-stepping algorithms.

Many problems describing multi-phase flows in porous media are convection dominated parabolic problems. When capillary forces are equal to zero the saturation equation in (2.16) becomes hyperbolic. Sharp fronts of solutions appear often in various applications. They should be resolved accurately by discrete schemes.

It is also very important to preserve the monotonicity of the solutions. Here we should balance between two possibilities. Upwind approximations

are monotone, but the approximation is only first order accurate. Centered differences are second order accurate but can yield oscillatory approximations if the solution is not smooth enough.

First order upwind discretizations are investigated in [4, 10, 17, 25]. A good review of upwind methods for conservation laws, including also a posteriori error estimates for upwind finite volume schemes is done by Kröner [21, 22].

Recently Tadmor *et al.* have proposed non-oscillatory central schemes for one-dimensional and multi-dimensional hyperbolic conservation laws [19, 20, 27], see also [23]. The main advantages of the proposed central schemes are the high resolution, due to the smaller amount of the numerical dissipation, and the simplicity. There are no Riemann solvers and characteristic decomposition involved. At the same time, the developed schemes have an upwind nature, since they respect the directions of wave propagation by measuring the one-sided local speeds. For some cases of schemes even the Jacobians associated with the problem are not required for the computations. The time integration is done by using the explicit predictor–corrector algorithm. Using similar ideas Balaguer and Conde proposed the fourth-order nonoscillatory upwind and central schemes for discretization of hyperbolic conservation laws [3].

In many papers splitting and decomposition methods are used to construct computationally efficient numerical algorithms:

a) Dimensional splitting is an effective method for solving multidimensional problems by constructing the integration algorithm from one-dimensional subproblems – one dimension at a time (see, e.g., [13, 25] or a classical book of Richtmayer and Morton [31]). In the context of nonlinear conservation laws this method is investigated by Crandal and Majda [12]. They proved that dimensional splitting encounters several limitations when applied for solving conservation laws.

b) Splitting in physical processes consists in solving separately a system of conservation laws (e.g. by applying an explicit scheme) and stiff diffusion and reaction problems (by using special implicit algorithms). Different time steps can be used for integration of each subproblem (see, e.g., [2]).

c) Local characteristic decomposition is used for the accurate resolution of complicated structure of solutions. The development of such methods started from the Godunov method, and now a large number of special classes of methods, e.g. ENO, WENO algorithms, are proposed (see, e.g. [25, 26, 30]). While this decomposition increases the computational cost, it controls spurious oscillations when the order of accuracy is high.

Our goal is to build a universal tool for solving a wide variety of problems of multiphase flows in porous media. Thus we have decided to start with not the most complicated but flexible and robust approximations. We try to avoid the time-consuming computation of approximate Riemann solvers and the related characteristic decompositions. Since dimensional splitting and splitting in physical processes also introduce numerical and non-physical errors, we avoid splitting also.

### 3.1. Finite volume discretization

We discretize equations (2.16) on structured nonuniform grids. A 2D space  $\Omega$  is used as an example in this section. We have a set of vertices:

$$V_h = \{v_{ij} = (x_{1i}, x_{2j}), \quad 0 \leq i \leq N_i, \quad 0 \leq j \leq N_j\}$$

where:

$$x_{1,i} = x_{1,i-1} + h_{1,i}, \quad x_{2,j} = x_{2,j-1} + h_{2,j}.$$

The grid  $V_h$  defines a structured mesh  $E_h$ , which covers the region  $\Omega$ :

$$E_h = \{e_{ij}, \quad 1 \leq i \leq N_i, \quad 1 \leq j \leq N_j\}.$$

Elements  $e_{ij}$  of the mesh are called cells or control volumes (thus, in fact we define a dual mesh in the terminology of [4]). In 2D we get *quadrilateral* elements. These elements can be *cell-centered* or *vertex-centered*. Our scheme is based on cell-centered mesh, and these vertices make a primary grid

$$\Omega_h = \{X_{ij}, \quad 1 \leq i \leq N_i, \quad 1 \leq j \leq N_j\}.$$

For boundary elements, one or more faces of which belong to the boundary  $\partial\Omega$ , the vertices are taken on the boundary. Let denote:

$$h_{1,i+1/2} = X_{i+1,j} - X_{ij}, \quad h_{2,j+1/2} = X_{i,j+1} - X_{ij}.$$

Based on the given grid we can define a finite dimensional function space of piecewise linear functions:

$$W_h = \{U(\mathbf{x}) : \quad U(\mathbf{x}) = \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} U_{ij} \varphi_{ij}(\mathbf{x})\}, \quad (3.1)$$

where  $\varphi_{ij}(\mathbf{x})$  are the usual nodal basis functions.

We describe the finite-volume scheme for the saturation equation, since the pressure equation is approximated in a similar way. Integrating the saturation equation (2.16) over the control element  $e \in E_h$  and applying the divergence theorem, we obtain

$$\int_e \varepsilon \frac{\partial(\rho_1 s_1)}{\partial t} d\mathbf{x} + \int_{\partial e} \left( \rho \mathbf{u} \lambda_1 + \frac{\mathbf{K} \lambda_1 \lambda_2}{\nu} (\nabla p_c + (\rho_1 - \rho_2) \mathbf{g}) \right) \cdot \mathbf{n} ds = 0.$$

The numerical diffusion flux over control element face is computed by using harmonic or arithmetic average of the diffusion coefficient. For example, in 2D case taking only one part of the element interface we get the following numerical diffusion flux:

$$\int_{\partial e_{i+1/2,j}} \frac{\mathbf{K} \lambda_1 \lambda_2}{\nu} \nabla p_c \cdot \mathbf{n} ds \approx h_{2j} \left( \frac{\mathbf{K} \lambda_1 \lambda_2}{\nu} \right)_{i+1/2,j} \frac{p_c(S_{i+1,j}) - p_c(S_{ij})}{h_{1,i+1/2}}.$$

The evaluation of the advective part of the flux is done by using the *fully upwinding* method

$$\int_{\partial e_{i+1/2,j}} \rho \mathbf{u} \lambda_1(S) \cdot \mathbf{n} ds \approx h_{2j} (\rho u_1)_{i+1/2,j} \cdot \begin{cases} \lambda_1(S_{ij}), & \text{if } \rho u_{1,i+1/2,j} \lambda'_1(S_{ij}) \geq 0, \\ \lambda(S_{i+1,j}), & \text{else.} \end{cases}$$

Fully upwinding discretization of the advective flux leads to positive diagonal and negative off-diagonal entries in the matrix obtained after linearization of nonlinear discrete equations by the Newton method and the discrete solution obeys a discrete maximum principle.

The drawback of such approximation is that artificial (numerical) diffusion is introduced. It can be split into two components: one along the streamline and a second component perpendicular to the streamline [17]. The second component exists only for multi – dimensional problems. A multidimensional-upwind method of first order is considered in [17], which try to reduce the grid orientation effects by taking into account the direction of the velocity field. Our strategy is to reduce the approximation error by decreasing the mesh step, since the obtained large systems of equations can be solved efficiently with parallel computers. For very fine mesh central differencing can be used also.

In our tool for 1D problems we have also implemented an explicit higher order TVD approximation of the advection flux, when the central difference approximation is combined with the upwind approximation by using the *minmod* limiter. Let consider the case, when  $\rho u_{1,i+1/2,j} \lambda'_1(S_{ij}) \geq 0$ , then the advection flux is approximated as follows

$$\int_{\partial e_{i+1/2,j}} \rho \mathbf{u} \lambda_1(S) \cdot \mathbf{n} ds \approx h_{2j} (\rho u_1)_{i+1/2,j} \lambda_1(S_{i+1/2,j}),$$

$$S_{i+1/2,j} = S_{ij} + \frac{h_{i+1/2,j}}{2} \minmod\left(\frac{S_{i+1,j} - S_{ij}}{h_{i+1/2,j}}, \frac{S_{ij} - S_{i-1,j}}{h_{i-1/2,j}}\right),$$

where the limiter is defined by

$$\minmod(a, b) = \begin{cases} a, & \text{if } ab > 0, \text{ and } |a| \leq |b|, \\ b, & \text{if } ab > 0, \text{ and } |b| \leq |a|, \\ 0, & \text{if } ab < 0. \end{cases}$$

After discretization the mass is conserved locally in each element and therefore the discrete problem satisfies the mass conservation property in the whole region  $\Omega$ .

### 3.2. Time-stepping algorithms

After approximation of space derivatives in system (2.16) a large system of nonstationary nonlinear DEs is obtained

$$\begin{cases} L_h(S)P(t) = F_p, \\ \frac{dS(t)}{dt} = C_h(S, P) + D_h(S) + F_s. \end{cases} \quad (3.2)$$

Here the first equation approximates the global pressure equation,  $C_h(S, P)$  denotes the convection part and  $D_h(S, P)$  the diffusion part of the semi-discrete saturation equation. We consider incompressible case. Let denote saturation and pressure values at time  $t^n$  by  $S^n$  and  $P^n$ , respectively.

The aim of time-stepping algorithms is to balance the stability and robustness of the integration algorithm with computational efficiency. The one way is to use a some kind of segregated solution procedure. With this approach the new pressure field  $P^{n+1}$  is computed first from

$$L_h(S^n)P^{n+1} = F_p^n, \quad (3.3)$$

which is a linear elliptic equation in  $P$  for a given saturation at previous time level  $t^n$ . Next, saturation at time level  $t^{n+1}$  is computed with a velocity field obtained from the new pressure field. The most simple way is to use the forward Euler scheme:

$$\frac{S^{n+1} - S^n}{\tau} = C_h(S^n, P^{n+1}) + D_h(S^n) + F_s^n. \quad (3.4)$$

This time-stepping procedure is named IMPES (for implicit pressure and explicit saturation). It was originally developed by Sheldon *et al.* [33] and Stone and Garder [34] for solving partial differential coupled system for two-phase flow in porous medium (see also [4, 17]). Due to the explicitness of the scheme for saturation equation IMPES is stable only when time steps are sufficiently small. An improved IMPES method which utilizes an adaptive control strategy for selection of time step is proposed in [9]. The stability of IMPES scheme for solving a three-phase flow problem is investigated in [11].

For many applications the strongest restriction on time step is due the diffusion part of saturation equation. The following implicit-explicit modification of (3.4) is used in some papers (see, e.g. [2]):

$$\frac{S^{n+1} - S^n}{\tau} = C_h(S^n, P^{n+1}) + D_h(S^{n+1}) + F_s^{n+1}, \quad (3.5)$$

which consists of applying an explicit discretization for the advection term and an implicit discretization for the diffusion and source terms. We note that the approximation of different terms on different time levels leads to truncation errors similar to additive scheme case. In fact scheme (3.5) is equivalent to the following splitting scheme

$$\begin{cases} \frac{S^{n+1/2} - S^n}{\tau} = C_h(S^n, P^{n+1}), \\ \frac{S^{n+1} - S^{n+1/2}}{\tau} = D_h(S^{n+1}) + F_s^{n+1}, \end{cases}$$

but the additive scheme is more flexible, since different time steps can be used for integration of each subproblem.

The next step to increase the stability of the discrete scheme is to use backward Euler (or more generally an implicit) integration method for the saturation equation:

$$\frac{S^{n+1} - S^n}{\tau} = C_h(S^{n+1}, P^{n+1}) + D_h(S^{n+1}) + F_s^{n+1}. \quad (3.6)$$

At each time level we get a nonlinear elliptic equation with advection-dominated space operator. It can be solved by some iterative procedure, e.g. the Newton method. The whole time-stepping procedure (3.3), (3.6) is named IMPIMS.

Another way is to use the coupled schemes. In our case, the *fully implicit/fully coupled* (FIFC) scheme gives the system

$$\begin{cases} L_h(S^{n+1})P^{n+1} = F_p^{n+1}, \\ \frac{S^{n+1} - S^n}{\tau} = C_h(S^{n+1}, P^{n+1}) + D_h(S^{n+1}, P^{n+1}) + F_s^{n+1}, \end{cases} \quad (3.7)$$

when both equations are solved simultaneously. The FIFC approach is usually selected for a maximum of robustness and stability. However, it can be very expensive computationally.

Our goal is to have a tool working with both: segregated and coupled solvers, to be able to choose the best for the specific problem. Currently, the IMPIMS type iterative algorithm is implemented in our tool with additional " $k$ "-iterations between separate equation solvers at each time level:

$$\begin{cases} L_h(S^{n+1,k})P^{n+1,k+1} = F_p^{n+1,k}, \\ \frac{S^{n+1,k+1} - S^n}{\tau} = C_h(S^{n+1,k+1}, P^{n+1,k+1}) + D_h(S^{n+1,k+1}) + F_s^{n+1,k+1}. \end{cases} \quad (3.8)$$

An quasi-Newton method is used to solve the nonlinear saturation equation. Let us write the diffusion term as

$$D_h(S) = \nabla_h \cdot (K(S) \nabla_h P_c(S)).$$

Let  $S^m = S^{n+1,k+1,m}$  denote the  $m$ -th iteration of quasi-Newton method. Then the next iterative approximation is defined as

$$S^{m+1} = S^m + S_\Delta^m,$$

where  $S_\Delta^m$  satisfies the following equation:

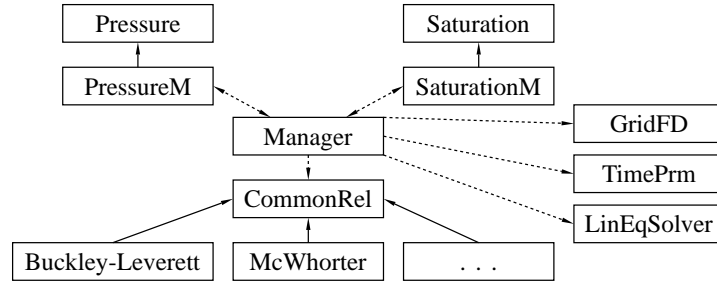
$$\begin{aligned} \frac{S_\Delta^m}{\tau} &= \partial C_h(S^m, P^{n+1,k+1}) S_\Delta^m + \nabla_h \cdot (K(S^m) P'_c(S^m) \nabla_h S_\Delta^m) + R^m, \\ R^m &= -\frac{S^m - S^n}{\tau} + C_h(S^m, P^{n+1,k+1}) + \nabla_h \cdot (K(S^m) \nabla_h P_c(S^m)) + F_s(S^m). \end{aligned}$$

#### 4. MfsolverC++: A Tool for Computations

Recently, it becomes very popular in the scientific computing to exploit the object-oriented programming (OOP) techniques. This allows developers to reduce the time spent on the programming and debugging and makes all implementation aspects cleaner and simpler.

We also use OOP in the design and implementation of our software tool **MfsolverC++** for computations of multiphase flows in porous media. We want to have a flexible set of efficient C++ modules to reduce the overhead for creation of different solvers for different schemes and problems.

Implementation of the solver for the solution of isothermal two-phase immiscible flow problems using global pressure model is shown in Figure 1. For this and other segregated solvers we use strategy proposed in [24] and used in *Diffpack* software library. According to it, solvers for the systems of PDEs are built by merging together the independent solvers for the alone-standing equations that enter the system.



**Figure 1.** Design of the PDE system solver with relations between solver classes, manager and pool of common relations. Solid arrows indicate inheritance ("is-a" relationship, with arrows pointing from subclass to base class). Dashed arrows indicate pointer ("has-a" relationship).

Class **Pressure** and his children are independent solvers of pressure equation (2.11). Class **Saturation** and his children are independent solvers of saturation equation (2.15). Equations become coupled into the system through the coefficients. In our PDE solvers, these coefficients, including the source, initial and boundary conditions functions, are represented by virtual functions. Subclasses of PDE solvers override these functions and implement the physically relevant versions, when the coefficients are coupled to other unknown fields in the PDE system. All these functions are often built of a common set of relations (constitutive relationships, model definitions, etc.). Therefore, they are collected in class hierarchies and accessed from PDE solvers through a base class **CommonRel** interface (pointer). Note that constitutive relationships can be easily changed without affecting the code in PDE solvers.

A class **Manager** acts as the solver class for the whole PDEs system and manages the whole solution of the given problem. This class contains two way

pointers to the subclasses for solving the pressure and saturation equations, `PressureM` and `SaturationM`, respectively, which enable the coupling by overriding the virtual functions of base classes with the functions from common relation hierarchy. The manager is also responsible for creating a space grid and time discretization. It allocates a common linear system and solver object, and distributes all these data to the PDE solver classes.

It is clear that segregated solvers have "implementational" advantage over coupled solvers. They are easier to implement, flexible and naturally extensible if the differential model is extended by additional PDEs.

Next we review very briefly some similar projects. First we mention a general PDE software tool *Diffpack*, which is an object oriented development framework for the solution PDE. It is a commercial product and many application examples are described in [24].

The toolbox UG is a framework for unstructured grid computations. Development of UG started in 1990 at the University of Heidelberg and proceeded at the University of Stuttgart from 1994. It is a flexible software tool for the numerical solution of partial differential equations on unstructured meshes in two and three space dimensions using multigrid methods.

A number of applications of this tool for computations of complex fluid flows in porous media are described in [5, 17]. For the time discretization either backward Euler, Crank-Nicholson or BDF(2) are used. The fully implicit/fully coupled time stepping strategy is selected for a maximum of robustness and stability. In UG the Newton method is used to solve large systems of nonlinear algebraic equations at each time step. The linear systems arising within the Newton method are solved with a multigrid method.

TOUGH2 is a general-purpose numerical simulation program for multiphase fluid and heat flow in porous and fractured media [29]. It is developed at Lawrence Berkeley National Laboratory and is widely used for computations on unstructured meshes (see e.g [28]).

In TOUGH2 code various strategies are implemented. In order to take into account the hyperbolic nature of the saturation equation very accurate explicit time-stepping algorithm TOUGH2-EOS3f with front tracking is used.

## 5. Computational Experiments

In this section we consider the injection process of carbone dioxide ( $CO_2$ ) into saline aquifers. Here an aqueous phase is displaced by a less dense and less viscous gas phase [28]. It is well known that immiscible displacement of a fluid by a less viscous one leads to the creation of fingers of low viscosity fluid penetrating the high viscosity fluid (see [18, 32]). On simulation level such phenomena arises due instabilities of macroscopic equations when the frontal mobility ratio is grater than one [4]. The appearance of finger-like structures can be triggered by

- numerical round-off errors,
- introducing a mild random variations of the permeability field.



We will note one more interesting aspect of this test problem (see [4, 15]). The phenomenon of viscous fingering comes from instabilities on *microscopic* level which are not modelled by the *macroscopic* equations, obtained after averaging process. Thus we can test a possibility to represent effects from smaller scale in a model on a larger scale. Numerical aspects of upscaling in simulation of flow porous media are investigated in [1, 8, 16].

The parameters of the model were taken from [28]. The capillary effects were assumed to be negligible. Then in fact the problem reduces to the Buckley - Leverett equation. Exactly this formulation was used in [28]. We describe the given problem in global pressure formulation and use a developed **MfsolverC++** tool. The most important coefficients are the relative permeability functions, which define the fractional flow function. The liquid is described by the van Genuchten function

$$k_{rl} = \sqrt{S^*} \left( 1 - (1 - (S^*)^{1/m})^m \right)^2, \quad S^* = \frac{S_l - S_{lr}}{1 - S_{lr}},$$

and the gas is described by the Brooks-Corey function:

$$k_{rg} = (1 - \hat{S})^2 (1 - \hat{S}^2), \quad \hat{S} = \frac{S_l - S_{lr}}{1 - S_{lr} - S_{gr}}.$$

For  $CO_2$  and water the viscosity was taken equal to  $\mu_g = 4 \cdot 10^{-5}$  and  $\mu_l = 7.5 \cdot 10^{-4}$ , respectively. The relative permeability parameters were defined as  $S_{lr} = 0.25$ ,  $S_{gr} = 0.05$ ,  $m = 0.85$ .

For the validation of the numerical discretizations and algorithms we solved one-dimensional case of this problem. Then a quasi-analytical solution is known (see [4, 17]) and thus it is possible to investigate the convergence of the numerical solution to the exact solution and to determine the experimental order of convergence.

The domain is discretized with  $N$  elements. The  $L_p$ -norms of the error in the saturation variable,

$$\|s_g - S_{gh}\|_{L_p} = \left( \int_{\Omega} |s_g - S_{gh}|^p \right)^{1/p},$$

are computed for  $p = 1, 2$ . The convergence rate  $r$  is determined as

$$r = \log \left( \frac{\|s_g - S_{gh}\|_{L_p}}{\|s_g - S_{g2h}\|_{L_p}} \right) / \log \frac{1}{2}.$$

Table 1 presents the error norms and the convergence rates for different numbers of the cells.

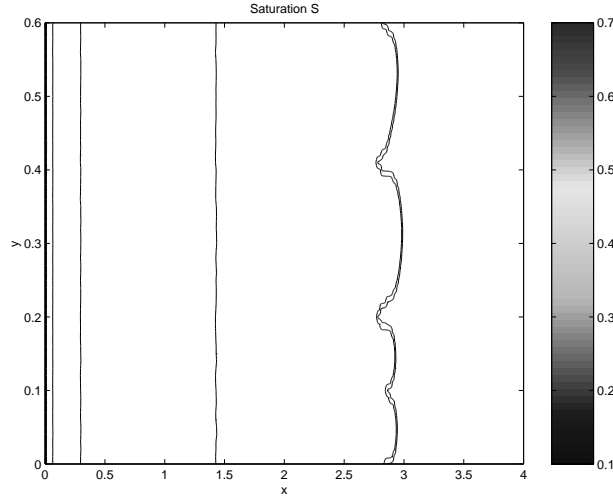
The results in table show that the experimental convergence rates are not reaching the optimal approximation orders of a step function with a linear spline, which are equal to  $\mathcal{O}(h)$  in the  $L_1$ -norm and  $\mathcal{O}(h^{1/2})$  in the  $L_2$ -norm.

The fingers were triggered by a random permeability field. We modified the permeability in the order of 5 %. It is well-known that the upwind discretization introduces a numerical diffusion, in order to reduce it the computations

**Table 1.** Experimental order of convergence for the 1D problem.

| N    | error $L_1$ | rate $L_1$ | error $L_2$ | rate $L_2$ |
|------|-------------|------------|-------------|------------|
| 65   | 0.1366      | 0.707      | 0.1023      | 0.391      |
| 129  | 0.0854      | 0.676      | 0.0786      | 0.380      |
| 257  | 0.0554      | 0.626      | 0.0605      | 0.377      |
| 513  | 0.0377      | 0.554      | 0.0466      | 0.378      |
| 1025 | 0.0274      | 0.463      | 0.0356      | 0.386      |

were done on very fine grids. Figure 2 shows the distribution of the gas saturation for one case of parameters. We have not investigated the convergence of the solution under grid refinement.

**Figure 2.** Distribution of gas saturation. Viscous fingers are triggered by the modified permeability field.

## Acknowledgements

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

## ***A Finite - Volume Particle Method for Compressible Flows***

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

(19 pages, 1998)

2. M. Feldmann, S. Seibold

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

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

*Keywords: Hilbert transform, damage diagnosis, Kalman filtering, non-linear dynamics*

(23 pages, 1998)

3. Y. Ben-Haim, S. Seibold

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

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

*Keywords: Robust reliability, convex models, Kalman filtering, multi-hypothesis diagnosis, rotating machinery, crack diagnosis*

(24 pages, 1998)

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

## ***Three-dimensional Radiative Heat Transfer in Glass Cooling Processes***

For the numerical simulation of 3D radiative heat transfer in glasses and glass melts, practically applicable mathematical methods are needed to handle such problems optimal using workstation class computers.

Since the exact solution would require super-computer capabilities we concentrate on approximate solutions with a high degree of accuracy. The following approaches are studied: 3D diffusion approximations and 3D ray-tracing methods.

(23 pages, 1998)

5. A. Klar, R. Wegener

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

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

(23 pages, 1998)

## ***Part II: Numerical and stochastic investigations***

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

(17 pages, 1998)

6. A. Klar, N. Siedow

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

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

(24 pages, 1998)

7. I. Choquet

## ***Heterogeneous catalysis modelling and numerical simulation in 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 gener-

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

(20 pages, 1998)

10. J. Mohring

## ***Helmholtz Resonators with Large Aperture***

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

(21 pages, 1998)

11. H. W. Hamacher, A. Schöbel

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

Finding “good” cycles in graphs is a problem of great interest in graph theory as well as in locational analysis. We show that the center and median problems are NP hard in general graphs. This result holds both for the variable cardinality case (i.e. all cycles of the graph are considered) and the fixed cardinality case (i.e. only cycles with a given cardinality  $p$  are feasible). Hence it is of interest to investigate special cases where the problem is solvable in polynomial time. In grid graphs, the variable cardinality case is, for instance, trivially solvable if the shape of the cycle can be chosen freely.

If the shape is fixed to be a rectangle one can analyze rectangles in grid graphs with, in sequence, fixed dimension, fixed cardinality, and variable cardinality. In all cases a complete characterization of the optimal cycles and closed form expressions of the optimal objective values are given, yielding polynomial time algorithms for all cases of center rectangle problems.

Finally, it is shown that center cycles can be chosen as rectangles for small cardinalities such that the center cycle problem in grid graphs is in these cases completely solved.

(15 pages, 1998)

12. H. W. Hamacher, K.-H. Küfer

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

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

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

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

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

(14 pages, 1999)

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

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

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

(20 pages, 1999)

14. M. Junk

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

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

are also applied to the construction of Chapman Enskog distributions which are used in Kinetic Schemes for compressible Navier-Stokes equations.

(24 pages, 1999)

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

### **A new discrete velocity method for Navier-Stokes equations**

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

(20 pages, 1999)

16. H. Neunzert

### **Mathematics as a Key to Key Technologies**

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

(39 pages (4 PDF-Files), 1999)

17. J. Ohser, K. Sandau

### **Considerations about the Estimation of the Size Distribution in Wickseil's Corpuscle Problem**

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

(18 pages, 1999)

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

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

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

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

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

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

**Keywords:** Continuous Location, Polyhedral Gauges, Finite Dominating Sets, Approximation, Sandwich Algorithm, Greedy Algorithm

(19 pages, 2000)

19. A. Becker

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

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

**Keywords:** Distortion measure, human visual system

(26 pages, 2000)

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

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

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

**Keywords:** integer programming, hub location, facility location, valid inequalities, facets, branch and cut

(21 pages, 2000)

21. H. W. Hamacher, A. Schöbel

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

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

(30 pages, 2001)

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

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

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

(16 pages, 2001)



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

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

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

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

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

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

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

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

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

approach. While most of the results are applicable to general evacuation situations, we concentrate on building evacuation.  
(44 pages, 2001)

25. J. Kuhnert, S. Tiwari

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

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

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

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

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

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

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

27. A. Zemitis

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

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

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

28. I. Ginzburg, K. Steiner

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

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

**Keywords:** Generalized LBE, free-surface phenomena,

interface boundary conditions, filling processes, Bingham viscoplastic model, regularized models  
(22 pages, 2001)

29. H. Neunzert

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

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

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

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

30. J. Kuhnert, S. Tiwari

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

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

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

31. R. Korn, M. Krekel

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

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

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

32. M. Krekel

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

If an investor borrows money he generally has to pay higher interest rates than he would have received, if he had put his funds on a savings account. The classical model of continuous time portfolio optimisation ignores this effect. Since there is obviously a connection between the default probability and the total per-

centage of wealth, which the investor is in debt, we study portfolio optimisation with a control dependent interest rate. Assuming a logarithmic and a power utility function, respectively, we prove explicit formulae of the optimal control.

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

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

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

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

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

34. I. Ginzburg, K. Steiner

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

A generalized lattice Boltzmann model to simulate free-surface is constructed in both two and three dimensions. The proposed model satisfies the interfacial boundary conditions accurately. A distinctive feature of the model is that the collision processes is carried out only on the points occupied partially or fully by the fluid. To maintain a sharp interfacial front, the method includes an anti-diffusion algorithm. The unknown distribution functions at the interfacial region are constructed according to the first order Chapman-Enskog analysis. The interfacial boundary conditions are satisfied exactly by the coefficients in the Chapman-Enskog expansion. The distribution functions are naturally expressed in the local interfacial coordinates. The macroscopic quantities at the interface are extracted from the least-square solutions of a locally linearized system obtained from the known distribution functions. The proposed method does not require any geometric front construction and is robust for any interfacial topology. Simulation results of realistic filling process are presented: rectangular cavity in two dimensions and Hammer box, Campbell box, Sheffield box, and Motorblock in three dimensions. To enhance the stability at high Reynolds numbers, various upwind-type schemes are developed. Free-slip and no-slip boundary conditions are also discussed.

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

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

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

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

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

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

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

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

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

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

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

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

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

38. D. d'Humières, I. Ginzburg

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

We present a unified approach of several boundary conditions for lattice Boltzmann models. Its general framework is a generalization of previously introduced schemes such as the bounce-back rule, linear or quadratic interpolations, etc. The objectives are two fold: first to give theoretical tools to study the existing boundary conditions and their corresponding accuracy; secondly to design formally third-order accurate boundary conditions for general flows. Using these boundary conditions, Couette and Poiseuille flows are exact solution of the lattice Boltzmann models for a Reynolds number  $Re = 0$  (Stokes limit). Numerical comparisons are given for Stokes flows in periodic arrays of spheres and cylinders, linear periodic array of cylinders between moving plates and for Navier-Stokes flows in periodic arrays of cylinders for  $Re < 200$ . These results show a significant improvement of the overall accuracy when using the linear interpolations instead of the bounce-back reflection (up to an order of magnitude on the hydrodynamics fields). Further improvement is achieved with the new multi-reflection boundary conditions, reaching a level of ac-

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

Finally the good stability of these schemes is highlighted by some simulations of moving obstacles: a cylinder between flat walls and a sphere in a cylinder.  
*Keywords: lattice Boltzmann equation, boundary conditions, bounce-back rule, Navier-Stokes equation*  
(72 pages, 2002)

39. R. Korn

### **Elementare Finanzmathematik**

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

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

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

### **Batch Presorting Problems: Models and Complexity Results**

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

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

41. J. Linn

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

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

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

42. T. Hanne, S. Nickel

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

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

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



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

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

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

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

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

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

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

44. T. Halfmann, T. Wichmann

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

Industrial analog circuits are usually designed using numerical simulation tools. To obtain a deeper circuit understanding, symbolic analysis techniques can additionally be applied. Approximation methods which reduce the complexity of symbolic expressions are needed in order to handle industrial-sized problems.

This paper will give an overview to the field of symbolic analog circuit analysis. Starting with a motivation, the state-of-the-art simplification algorithms for linear as well as for nonlinear circuits are presented. The basic ideas behind the different techniques are described, whereas the technical details can be found in the cited references. Finally, the application of linear and nonlinear symbolic analysis will be shown on two example circuits.

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

45. S. E. Mikhailov, J. Orlik

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

Asymptotic homogenisation technique and two-scale convergence is used for analysis of macro-strength and fatigue durability of composites with a periodic structure under cyclic loading. The linear damage accumulation rule is employed in the 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 & Mladenović [HM97] for the p-median problem is described. An extensive numerical study is presented to show the efficiency of both heuristics and compare them.

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

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

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

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

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

48. S. Feldmann, P. Lang

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

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

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

49. J. Kallrath, S. Nickel

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

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

the BPSP. Competitive analysis is used for comparing the algorithms.

**Keywords:** *batch presorting problem, online optimization, competitive analysis, polynomial algorithms, logistics* (17 pages, 2003)

50. T. Hanne, H. L. Trinka

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

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

**Key words:** *Multicriteria decision making, knowledge management, decision support systems, visual interfaces, interactive navigation, real-life applications.* (26 pages, 2003)

51. O. Iliev, V. Laptev

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

This paper concerns numerical simulation of flow through oil filters. Oil filters consist of filter housing (filter box), and a porous filtering medium, which completely separates the inlet from the outlet. We discuss mathematical models, describing coupled flows in the pure liquid subregions and in the porous filter media, as well as interface conditions between them. Further, we reformulate the problem in fictitious regions method manner, and discuss peculiarities of the numerical algorithm in solving the coupled system. Next, we show numerical results, validating the model and the algorithm. Finally, we present results from simulation of 3-D oil flow through a real car filter.

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

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

#### **On a Multigrid Adaptive Refinement Solver for Saturated Non-Newtonian Flow in Porous Media**

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

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

53. S. Kruse

#### **On the Pricing of Forward Starting Options under Stochastic Volatility**

We consider the problem of pricing European forward starting options in the presence of stochastic volatility. By performing a change of measure using the asset

price at the time of strike determination as a numeraire, we derive a closed-form solution based on Heston's model of stochastic volatility.

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

54. O. Iliev, D. Stoyanov

#### **Multigrid – adaptive local refinement solver for incompressible flows**

A non-linear multigrid solver for incompressible Navier-Stokes equations, exploiting finite volume discretization of the equations, is extended by adaptive local refinement. The multigrid is the outer iterative cycle, while the SIMPLE algorithm is used as a smoothing procedure. Error indicators are used to define the refinement subdomain. A special implementation approach is used, which allows to perform unstructured local refinement in conjunction with the finite volume discretization.

The multigrid - adaptive local refinement algorithm is tested on 2D Poisson equation and further is applied to a lid-driven flows in a cavity (2D and 3D case), comparing the results with bench-mark data. The software design principles of the solver are also discussed.

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

55. V. Starikovicius

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

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

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

56. P. Lang, A. Sarishvili, A. Wirsén

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

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

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

57. H. Knaf, P. Lang, S. Zeiser

#### **Diagnosis aiding in Regulation Thermography using Fuzzy Logic**

The objective of the present article is to give an overview of an application of Fuzzy Logic in Regulation

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

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

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

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

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

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

59. J. Orlik

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

We consider the contact of two elastic bodies with rough surfaces at the interface. The size of the micro-peaks and valleys is very small compared with the macro-size 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 contradictory goals of delivering a sufficiently high dose to the target while widely sparing critical structures. The search for this a priori unknown compromise typically requires the computation of several plans, i.e. the solution of several optimization problems. This accumulates to a high computational expense due to the large scale of these problems – a consequence of the discrete problem formulation. This paper presents the adaptive clustering method as a new algorithmic concept to overcome these difficulties. The computations are performed on an individually adapted structure of voxel clusters rather than on the original voxels leading to a decisively reduced computational complexity as numerical examples on real clinical data demonstrate. In contrast to many other similar concepts, the typical trade-off between a reduction in computational complexity and a loss in exactness can

be avoided: the adaptive clustering method produces the optimum of the original problem. This flexible method can be applied to both single- and multi-criteria optimization methods based on most of the convex evaluation functions used in practice.

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

61. D. Kehrwald

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

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

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

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

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

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

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

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

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

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

We also solve an inverse problem and present algorithms for the determination of the absolute preform permeability coefficient in the case when the velocity of the penetration front is known from measurements. In both cases (direct and inverse problems) we emphasize on the specifics related to the non-Newtonian behavior of the polymer. For completeness, we discuss also the Newtonian case. Results of some experimental

measurements are presented and discussed.

**Keywords:** *Liquid Polymer Moulding, Modelling, Simulation, Infiltration, Front Propagation, non-Newtonian flow in porous media*  
(43 pages, 2004)

64. T. Hanne, H. Neu

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

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

**Keywords:** *Human resource modeling, software process, productivity, human factors, learning curve*  
(14 pages, 2004)

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

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

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

**Keywords:** *fluid-structure interaction, deformable porous media, upscaling, linear elasticity, stokes, finite elements*  
(28 pages, 2004)

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

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

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

**Keywords:** *poroelasticity, multilayered material, finite volume discretization, MAC type grid*  
(41 pages, 2004)

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

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

A spectral theory for constituents of macroscopically homogeneous random microstructures modeled as homogeneous random closed sets is developed and provided with a sound mathematical basis, where the spectrum obtained by Fourier methods corresponds to

the angular intensity distribution of x-rays scattered by this constituent. It is shown that the fast Fourier transform applied to three-dimensional images of microstructures obtained by micro-tomography is a powerful tool of image processing. The applicability of this technique is demonstrated in the analysis of images of porous media.

**Keywords:** *porous microstructure, image analysis, random set, fast Fourier transform, power spectrum, Bartlett spectrum*  
(13 pages, 2004)

68. H. Neunzert

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

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

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

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

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

**Keywords:** *poroelasticity, multilayered material, finite volume discretizations, MAC type grid, error estimates*  
(26 pages, 2004)

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

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

Flow of non-Newtonian in saturated porous media can be described by the continuity equation and the generalized Darcy law. Efficient solution of the resulting second order nonlinear elliptic equation is discussed here. The equation is discretized by a finite volume method on a cell-centered grid. Local adaptive refinement of the grid is introduced in order to reduce the number of unknowns. A special implementation approach is

used, which allows us to perform unstructured local refinement in conjunction with the finite volume discretization. Two residual based error indicators are exploited in the adaptive refinement criterion. Second order accurate discretization on the interfaces between refined and non-refined subdomains, as well as on the boundaries with Dirichlet boundary condition, are presented here, as an essential part of the accurate and efficient algorithm. A nonlinear full approximation storage multigrid algorithm is developed especially for the above described composite (coarse plus locally refined) grid approach. In particular, second order approximation around interfaces is a result of a quadratic approximation of slave nodes in the multigrid - adaptive refinement (MG-AR) algorithm. Results from numerical solution of various academic and practice-induced problems are presented and the performance of the solver is discussed.

**Keywords:** *Nonlinear multigrid, adaptive refinement, non-Newtonian in porous media*  
(25 pages, 2004)

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

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

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

**Keywords:** *territory design, political districting, sales territory alignment, optimization algorithms, Geographical Information Systems*  
(40 pages, 2005)

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

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

In order to optimize the acoustic properties of a stacked fiber non-woven, the microstructure of the non-woven is modeled by a macroscopically homogeneous random system of straight cylinders (tubes). That is, the fibers are modeled by a spatially stationary random system of lines (Poisson line process), dilated by a sphere. Pressing the non-woven causes anisotropy. In our model, this anisotropy is described by a one parametric distribution of the direction of the fibers. In the present application, the anisotropy parameter has to be estimated from 2d reflected light microscopic images of microsections of the non-woven.

After fitting the model, the flow is computed in digitized realizations of the stochastic geometric model using the lattice Boltzmann method. Based on the flow resistivity, the formulas of Delany and Bazley predict the frequency-dependent acoustic absorption of the non-woven in the impedance tube.

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

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



73. V. Rutka, A. Wiegmann

**Explicit Jump Immersed Interface Method for virtual material design of the effective elastic moduli of composite materials**

Virtual material design is the microscopic variation of materials in the computer, followed by the numerical evaluation of the effect of this variation on the material's macroscopic properties. The goal of this procedure is an in some sense improved material. Here, we give examples regarding the dependence of the effective elastic moduli of a composite material on the geometry of the shape of an inclusion. A new approach on how to solve such interface problems avoids mesh generation and gives second order accurate results even in the vicinity of the interface.

The Explicit Jump Immersed Interface Method is a finite difference method for elliptic partial differential equations that works on an equidistant Cartesian grid in spite of non-grid aligned discontinuities in equation parameters and solution. Near discontinuities, the standard finite difference approximations are modified by adding correction terms that involve jumps in the function and its derivatives. This work derives the correction terms for two dimensional linear elasticity with piecewise constant coefficients, i. e. for composite materials. It demonstrates numerical convergence and approximation properties of the method.

**Keywords:** virtual material design, explicit jump immersed interface method, effective elastic moduli, composite materials  
(22 pages, 2005)

74. T. Hanne

**Eine Übersicht zum Scheduling von Baustellen**

Im diesem Dokument werden Aspekte der formalen zeitlichen Planung bzw. des Scheduling für Bauprojekte anhand ausgewählter Literatur diskutiert. Auf allgemeine Aspekte des Scheduling soll dabei nicht eingegangen werden. Hierzu seien als Standard-Referenzen nur Brucker (2004) und Pinedo (1995) genannt. Zu allgemeinen Fragen des Projekt-Managements sei auf Kerzner (2003) verwiesen.

Im Abschnitt 1 werden einige Anforderungen und Besonderheiten der Planung von Baustellen diskutiert. Diese treten allerdings auch in zahlreichen anderen Bereichen der Produktionsplanung und des Projektmanagements auf. In Abschnitt 2 werden dann Aspekte zur Formalisierung von Scheduling-Problemen in der Bauwirtschaft diskutiert, insbesondere Ziele und zu berücksichtigende Restriktionen. Auf eine mathematische Formalisierung wird dabei allerdings verzichtet. Abschnitt 3 bietet eine Übersicht über Verfahren und grundlegende Techniken für die Berechnung von Schedules. In Abschnitt 4 wird ein Überblick über vorhandene Software, zum einen verbreitete Internationale Software, zum anderen deutschsprachige Branchenlösungen, gegeben. Anschließend werden Schlussfolgerungen gezogen und es erfolgt eine Auflistung der Literaturquellen.

**Keywords:** Projektplanung, Scheduling, Bauplanung, Bauindustrie  
(32 pages, 2005)

75. J. Linn

**The Folgar–Tucker Model as a Differential Algebraic System for Fiber Orientation Calculation**

The Folgar–Tucker equation (FTE) is the model most frequently used for the prediction of fiber orientation (FO) in simulations of the injection molding process for short-fiber reinforced thermoplasts. In contrast to its widespread use in injection molding simulations, little is known about the mathematical properties of the FTE: an investigation of e. g. its phase space  $M_{FT}$  has been presented only recently [12]. The restriction of the dependent variable of the FTE to the set  $M_{FT}$  turns the FTE into a differential algebraic system (DAS), a fact which is commonly neglected when devising numerical schemes for the integration of the FTE. In this article we present some recent results on the problem of trace stability as well as some introductory material which complements our recent paper [12].

**Keywords:** fiber orientation, Folgar–Tucker model, invariants, algebraic constraints, phase space, trace stability  
(15 pages, 2005)

76. M. Speckert, K. Dreßler, H. Mauch, A. Lion, G. J. Wierda

**Simulation eines neuartigen Prüfsystems für Achserproben durch MKS-Modellierung einschließlich Regelung**

Testing new suspensions based on real load data is performed on elaborate multi channel test rigs. Usually, wheel forces and moments measured during driving maneuvers are reproduced by the test rig. Because of the complicated interaction between test rig and suspension each new rig configuration has to prove its efficiency with respect to the requirements and the configuration might be subject to optimization.

This paper deals with mathematical and physical modeling of a new concept of a test rig which is based on two hexapods. The model contains the geometric configuration as well as the hydraulics and the controller. It is implemented as an ADAMS/Car template and can be combined with different suspension models to get a complete assembly representing the entire test rig. Using this model, all steps required for a real test run such as controller adaptation, drive file iteration and simulation can be performed. Geometric or hydraulic parameters can be modified easily to improve the setup and adapt the system to the suspension and the given load data.

The model supports and accompanies the introduction of the new rig concept and can be used to prepare real tests on a virtual basis. Using both a front and a rear suspension the approach is described and the potentials coming with the simulation are pointed out.

**Keywords:** virtual test rig, suspension testing, multi-body simulation, modeling hexapod test rig, optimization of test rig configuration  
(20 pages, 2005)

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77. K.-H. Küfer, M. Monz, A. Scherrer, P. Süß, F. Alonso, A. S. A. Sultan, Th. Bortfeld, D. Craft, Chr. Thieke

**Multicriteria optimization in intensity modulated radiotherapy planning**

Inverse treatment planning of intensity modulated radiotherapy is a multicriteria optimization problem: planners have to find optimal compromises between a sufficiently highdose intumor tissue that guarantee a high tumor control, and, dangerous overdosing of critical structures, in order to avoid high normal tissue complication problems.

The approach presented in this work demonstrates how to state a flexible generic multicriteria model of the IMRT planning problem and how to produce clinically highly relevant Pareto-solutions. The model is imbedded in a principal concept of Reverse Engineering, a general optimization paradigm for design problems. Relevant parts of the Pareto-set are approximated by using extreme compromises as cornerstone solutions, a concept that is always feasible if box constraints for objective functions are available. A major practical drawback of generic multicriteria concepts trying to compute or approximate parts of the Pareto-set is the high computational effort. This problem can be overcome by exploitation of an inherent asymmetry of the IMRT planning problem and an adaptive approximation scheme for optimal solutions based on an adaptive clustering preprocessing technique. Finally, a coherent approach for calculating and selecting solutions in a real-timeinteractive decision-making process is presented. The paper is concluded with clinical examples and a discussion of ongoing research topics.

**Keywords:** multicriteria optimization, extreme solutions, real-time decision making, adaptive approximation schemes, clustering methods, IMRT planning, reverse engineering  
(51 pages, 2005)

78. S. Amstutz, H. Andrä

**A new algorithm for topology optimization using a level-set method**

The levelset method has been recently introduced in the field of shape optimization, enabling a smooth representation of the boundaries on a fixed mesh and therefore leading to fast numerical algorithms. However, most of these algorithms use a HamiltonJacobi

equation to connect the evolution of the levelset function with the deformation of the contours, and consequently they cannot create any new holes in the domain (at least in 2D). In this work, we propose an evolution equation for the levelset function based on a generalization of the concept of topological gradient. This results in a new algorithm allowing for all kinds of topology changes.

**Keywords:** shape optimization, topology optimization, topological sensitivity, level-set  
(22 pages, 2005)

79. N. Ettrich

**Generation of surface elevation models for urban drainage simulation**

Traditional methods fail for the purpose of simulating the complete flow process in urban areas as a consequence of heavy rainfall and as required by the European Standard EN-752 since the bi-directional coupling between sewer and surface is not properly handled. The methodology, developed in the BMBF/EUREKA-project RiUrSim, solves this problem by carrying out the runoff on the basis of shallow water equations solved on high-resolution surface grids. Exchange nodes between the sewer and the surface, like inlets and manholes, are located in the computational grid and water leaving the sewer in case of surcharge is further distributed on the surface.

So far, it has been a problem to get the dense topographical information needed to build models suitable for hydrodynamic runoff calculation in urban areas. Recent airborne data collection methods like laser scanning, however, offer a great chance to economically gather densely sampled input data. This paper studies the potential of such laser-scan data sets for urban water hydrodynamics.

**Keywords:** Flooding, simulation, urban elevation models, laser scanning  
(22 pages, 2005)

80. H. Andrä, J. Linn, I. Matei, I. Shklyar, K. Steiner, E. Teichmann

**OPTCAST – Entwicklung adäquater Strukturoptimierungsverfahren für Gießereien Technischer Bericht (KURZFASSUNG)**

Im vorliegenden Bericht werden die Erfahrungen und Ergebnisse aus dem Projekt OptCast zusammengestellt. Das Ziel dieses Projekts bestand (a) in der Anpassung der Methodik der automatischen Strukturoptimierung für Gussteile und (b) in der Entwicklung und Bereitstellung von gießereispezifischen Optimierungstools für Gießereien und Ingenieurbüros.

Gießtechnische Restriktionen lassen sich nicht auf geometrische Restriktionen reduzieren, sondern sind nur über eine Gießsimulation (Erstarrungssimulation und Eigenspannungsanalyse) adäquat erfassbar, da die lokalen Materialeigenschaften des Gussteils nicht nur von der geometrischen Form des Teils, sondern auch vom verwendeten Material abhängen. Wegen dieser Erkenntnis wurde ein neuartiges iteratives Topologieoptimierungsverfahren unter Verwendung der Level-Set-Technik entwickelt, bei dem keine variable Dichte des Materials eingeführt wird. In jeder Iteration wird ein scharfer Rand des Bauteils berechnet. Somit ist die Gießsimulation in den iterativen Optimierungsprozess integrierbar.

Der Bericht ist wie folgt aufgebaut: In Abschnitt 2 wird der Anforderungskatalog erläutert, der sich aus der Bearbeitung von Benchmark-Problemen in der ersten Projektphase ergab. In Abschnitt 3 werden die Benchmark-Probleme und deren Lösung mit den im Projekt entwickelten Tools beschrieben. Abschnitt 4 enthält die Beschreibung der neu entwickelten Schnittstellen und die mathematische Formulierung des Topologieoptimierungsproblems. Im letzten Abschnitt wird das neue Topologieoptimierungsverfahren, das die Simulation des Gießprozesses einschließt, erläutert.

**Keywords:** Topologieoptimierung, Level-Set-Methode, Gießprozesssimulation, Gießtechnische Restriktionen, CAE-Kette zur Strukturoptimierung  
(77 pages, 2005)

81. N. Marheineke, R. Wegener

### **Fiber Dynamics in Turbulent Flows Part I: General Modeling Framework**

The paper at hand deals with the modeling of turbulence effects on the dynamics of a long slender elastic fiber. Independent of the choice of the drag model, a general aerodynamic force concept is derived on the basis of the velocity field for the randomly fluctuating component of the flow. Its construction as centered differentiable Gaussian field complies thereby with the requirements of the stochastic  $k$ - $\epsilon$  turbulence model and Kolmogorov's universal equilibrium theory on local isotropy.

**Keywords:** fiber-fluid interaction; Cosserat rod; turbulence modeling; Kolmogorov's energy spectrum; double-velocity correlations; differentiable Gaussian fields

### **Part II: Specific Taylor Drag**

In [12], an aerodynamic force concept for a general air drag model is derived on top of a stochastic  $k$ - $\epsilon$  description for a turbulent flow field. The turbulence effects on the dynamics of a long slender elastic fiber are particularly modeled by a correlated random Gaussian force and in its asymptotic limit on a macroscopic fiber scale by Gaussian white noise with flow-dependent amplitude. The paper at hand now presents quantitative similarity estimates and numerical comparisons for the concrete choice of a Taylor drag model in a given application.

**Keywords:** flexible fibers;  $k$ - $\epsilon$  turbulence model; fiber-turbulence interaction scales; air drag; random Gaussian aerodynamic force; white noise; stochastic differential equations; ARMA process (38 pages, 2005)

82. C. H. Lampert, O. Wirjadi

### **An Optimal Non-Orthogonal Separation of the Anisotropic Gaussian Convolution Filter**

We give an analytical and geometrical treatment of what it means to separate a Gaussian kernel along arbitrary axes in  $\mathbb{R}^n$ , and we present a separation scheme that allows to efficiently implement anisotropic Gaussian convolution filters in arbitrary dimension. Based on our previous analysis we show that this scheme is optimal with regard to the number of memory accesses and interpolation operations needed.

Our method relies on non-orthogonal convolution axes and works completely in image space. Thus, it avoids the need for an FFT-subroutine. Depending on the accuracy and speed requirements, different interpolation schemes and methods to implement the one-dimensional Gaussian (FIR, IIR) can be integrated. The algorithm is also feasible for hardware that does not contain a floating-point unit.

Special emphasis is laid on analyzing the performance and accuracy of our method. In particular, we show that without any special optimization of the source code, our method can perform anisotropic Gaussian filtering faster than methods relying on the Fast Fourier Transform.

**Keywords:** Anisotropic Gaussian filter, linear filtering, orientation space,  $nD$  image processing, separable filters (25 pages, 2005)

83. H. Andrä, D. Stoyanov

### **Error indicators in the parallel finite element solver for linear elasticity DDFEM**

This report discusses two approaches for a posteriori error indication in the linear elasticity solver DDFEM: An indicator based on the Richardson extrapolation and Zienkiewicz-Zhu-type indicator.

The solver handles 3D linear elasticity steady-state problems. It uses own input language to describe the mesh and the boundary conditions. Finite element discretization over tetrahedral meshes with first or second order shape functions (hierarchical basis) has been used to resolve the model. The parallelization of the numerical method is based on the domain decomposition approach. DDFEM is highly portable over a set of parallel computer architectures supporting the MPI-standard.

**Keywords:** linear elasticity, finite element method, hierarchical shape functions, domain decomposition, parallel implementation, a posteriori error estimates (21 pages, 2006)

84. M. Schröder, I. Solchenbach

### **Optimization of Transfer Quality in Regional Public Transit**

In this paper we address the improvement of transfer quality in public mass transit networks. Generally there are several transit operators offering service and our work is motivated by the question how their timetables can be altered to yield optimized transfer possibilities in the over-all network. To achieve this, only small changes to the timetables are allowed.

The set-up makes it possible to use a quadratic semi-assignment model to solve the optimization problem. We apply this model, equipped with a new way to assess transfer quality, to the solution of four real-world examples. It turns out that improvements in overall transfer quality can be determined by such optimization-based techniques. Therefore they can serve as a first step towards a decision support tool for planners of regional transit networks.

**Keywords:** public transit, transfer quality, quadratic assignment problem (16 pages, 2006)

85. A. Naumovich, F. J. Gaspar

### **On a multigrid solver for the three-dimensional Biot poroelasticity system in multi-layered domains**

In this paper, we present problem-dependent prolongation and problem-dependent restriction for a multigrid solver for the three-dimensional Biot poroelasticity system, which is solved in a multilayered domain. The system is discretized on a staggered grid using the finite volume method. During the discretization, special care is taken of the discontinuous coefficients. For the efficient multigrid solver, a need in operator-dependent restriction and/or prolongation arises. We derive these operators so that they are consistent with the discretization. They account for the discontinuities of the coefficients, as well as for the coupling of the unknowns within the Biot system. A set of numerical experiments shows necessity of use of the operator-dependent restriction and prolongation in the multigrid solver for the considered class of problems.

**Keywords:** poroelasticity, interface problem, multigrid, operator-dependent prolongation (11 pages, 2006)

86. S. Panda, R. Wegener, N. Marheineke

### **Slender Body Theory for the Dynamics of Curved Viscous Fibers**

The paper at hand presents a slender body theory for the dynamics of a curved inertial viscous Newtonian fiber. Neglecting surface tension and temperature dependence, the fiber flow is modeled as a three-dimensional free boundary value problem via instantaneous incompressible Navier-Stokes equations. From regular asymptotic expansions in powers of the slenderness parameter leading-order balance laws for mass (cross-section) and momentum are derived that combine the unrestricted motion of the fiber center-line with the inner viscous transport. The physically reasonable form of the one-dimensional fiber model results thereby from the introduction of the intrinsic velocity that characterizes the convective terms.

**Keywords:** curved viscous fibers; fluid dynamics; Navier-Stokes equations; free boundary value problem; asymptotic expansions; slender body theory (14 pages, 2006)

87. E. Ivanov, H. Andrä, A. Kudryavtsev

### **Domain Decomposition Approach for Automatic Parallel Generation of Tetrahedral Grids**

The desire to simulate more and more geometrical and physical features of technical structures and the availability of parallel computers and parallel numerical solvers which can exploit the power of these machines have lead to a steady increase in the number of grid elements used. Memory requirements and computational time are too large for usual serial PCs. An a priori partitioning algorithm for the parallel generation of 3D nonoverlapping compatible unstructured meshes based on a CAD surface description is presented in this paper. Emphasis is given to practical issues and implementation rather than to theoretical complexity. To achieve

robustness of the algorithm with respect to the geometrical shape of the structure authors propose to have several or many but relatively simple algorithmic steps. The geometrical domain decomposition approach has been applied. It allows us to use classic 2D and 3D high-quality Delaunay mesh generators for independent and simultaneous volume meshing. Different aspects of load balancing methods are also explored in the paper. The MPI library and SPMD model are used for parallel grid generator implementation. Several 3D examples are shown.

**Key words:** Grid Generation, Unstructured Grid, Delaunay Triangulation, Parallel Programming, Domain Decomposition, Load Balancing (18 pages, 2006)

88. S. Tiwari, S. Antonov, D. Hietel, J. Kuhnert, R. Wegener

### **A Meshfree Method for Simulations of Interactions between Fluids and Flexible Structures**

We present the application of a meshfree method for simulations of interaction between fluids and flexible structures. As a flexible structure we consider a sheet of paper. In a twodimensional framework this sheet can be modeled as curve by the dynamical Kirchhoff-Love theory. The external forces taken into account are gravitation and the pressure difference between upper and lower surface of the sheet. This pressure difference is computed using the Finite Pointset Method (FPM) for the incompressible Navier-Stokes equations. FPM is a meshfree, Lagrangian particle method. The dynamics of the sheet are computed by a finite difference method. We show the suitability of the meshfree method for simulations of fluidstructure interaction in several applications

**Key words:** Meshfree Method, FPM, Fluid Structure Interaction, Sheet of Paper, Dynamical Coupling (16 pages, 2006)

89. R. Ciegis, O. Iliev, V. Starikovicius, K. Steiner

### **Numerical Algorithms for Solving Problems of Multiphase Flows in Porous Media**

In this paper we discuss numerical algorithms for solving the system of nonlinear PDEs, arising in modelling of two-phase flows in porous media, as well as the proper object oriented implementation of these algorithms. Global pressure model for isothermal two-phase immiscible flow in porous media is considered in this paper. Finite-volume method is used for the space discretization of the system of PDEs. Different time stepping discretizations and linearization approaches are discussed. The main concepts of the PDE software tool MfsolverC++ are given. Numerical results for one realistic problem are presented.

**Keywords:** nonlinear algorithms, finite-volume method, software tools, porous media, flows (16 pages, 2006)

90. D. Niedziela, O. Iliev, A. Latz

### **On 3D Numerical Simulations of Viscoelastic Fluids**

In this work we present and solve a class of non-Newtonian viscoelastic fluid flow problems. Models for non-Newtonian fluids can be classified into three large groups depending on the type of the constitutive relation used: algebraic, differential and integral. The first type of models are most simple one, the last are the most physically adequate ones. Here we consider some models from the first and the third groups, and present robust and efficient algorithms for their solution. We present new mathematical model, which belongs to the class of generalized Newtonian models and is able to account for the anisotropy of the viscosity tensor observed in many real liquids. In particular, we discuss a unified model that captures both shear thinning and extensional thickening for complex flows. The resulting large variations of the viscosity tensor in space and time are leading to a strong numerical coupling of the momentum equations due to the appearance of mixed derivatives in the discretization. To treat this strong coupling appropriately, we present two modifications of classical projection methods (like e.g. SIMPLE). In the first modification all momentum equations are solved coupled (i.e. mixed derivative are discretized implicitly) but still iterations are performed between the momen-

tum equations and the continuity equation. The second one is a fully coupled method, where momentum and continuity equation are solved together using a proper preconditioner. The models involving integral constitutive relation which accounts for the history of deformations, result in a system of integro-differential equations. To solve it, we suggest a proper splitting scheme, which treats the integral and the differential parts consecutively. Integral Oldroyd B and Doi Edwards models are used to simulate flows of dilute and concentrated polymer solutions, respectively.

*Keywords: non-Newtonian fluids, anisotropic viscosity, integral constitutive equation*  
(18 pages, 2006)

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