Fraunhofer Institut
Techno- und
Wirtschaftsmathematik

J. Kuhnert, S. Tiwari

Grid free method for solving the Poisson equation

Berichte des Fraunhofer ITWM, Nr. 25 (2001)

ISSN 1434-9973

Bericht 25 (2001)

Die Veröffentlichungen in der Berichtsreihe des Fraunhofer ITWM können bezogen werden über:

Fraunhofer-Institut für Techno- und
Wirtschaftsmathematik ITWM
Gottlieb-Daimler-Straße, Geb. 49

67663 Kaiserslautern

Telefon: +49 (0) 6 31/2 05-32 42
Telefax: +49 (0) 6 31/2 05-41 39
E-Mail: info@itwm.fhg.de
Internet: www.itwm.fhg.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.

Prof. Dr. Dieter Prätzel-Wolters
Institutsleiter

Kaiserslautern, im Juni 2001

Grid free method for solving the Poisson equation

S. Tiwari *, J. Kuhnert
Fraunhofer Institut Techno- und Wirtschaftmathematik
Gottlieb-Daimler-Strasse
Gebäude 49
D-67663 Kaiserslautern, Germany

Abstract

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

1. Introduction

Grid free methods are originally developed to simulate fluid dynamic problems. They are so called particle methods. A computational domain or fluid is replaced by a discrete set of points or particles and they move with the fluid. Initially, the so-called smoothed particle hydrodynamics (SPH), was developed to solve astrophysical problems without boundary [7, 5]. The method of SPH has been extended to solve various problems in fluid dynamics, see [8, 9, 10, 11] for further references.

Another grid free method for solving fluid dynamic problems is based on the least squares or moving least squares method [3, 4, 1, 6, 12, 13, 14]. The basic idea of this method is to approximate spatial derivatives of a function at an arbitrary point from the values on the surrounding cloud of points. These points need not to be regularly distributed and can be quite arbitrary.

The solution of the Poisson equation is necessary for instationary problems in incompressible fluid flows. Here, one considers some projection methods for the Navier-Stokes equations, where the Poisson equation for the pressure has to be solved [2]. Several authors have considered the projection method on grid based structure such that the Poisson equation can be solved by standard

* Supported by DFG - Priority Research Program: Analysis and Numerics for Conservation Laws.

methods like the finite element or the finite difference method. The grid based method can be quite complicated if the computational domain changes in time or takes complicated shapes. In this case, remeshing is required and more computational effort is needed. Therefore, a grid free method has certainly advantages in such cases. But, the standard Poisson solver cannot directly be applied on irregular grids.

The main motivation of this work is to solve the Poisson equation in a grid free structure such that it can be used in Lagrangian particle projection methods for incompressible flows. The method can be applied to any elliptic problem. It is suitable for a numerical solution of an elliptic equation in complicated geometry where the mesh is poorly constructed.

Our method is a local iteration process. It is based on the least squares approximation. A function and its derivatives can be very accurately approximated by the least squares method at an arbitrary point from its discrete values belonging to the surrounding cloud of points. However, the values of a function on the particle position is not given. Only the Passion equation is given. Therefore, we prescribe an initial guess for the values of a function on each particle position. In every iteration step, we enforce the Poisson equation to be satisfied on each particle in the least squares ansatz.

The boundary conditions can easily be handled. Boundaries can be replaced by a discrete set of boundary particles. For the Dirichlet boundary condition, boundary values are assigned in every iteration step, on boundary particles. For the Neumann boundary condition, we again enforce it to be satisfied in the least squares ansatz. Therefore, we add one more additional equation in the least squares approximation.

The method is stable and the numerical solution converges to a unique fixed point as the number of iteration steps tends to infinity. The method can be applied to coarser as well as finer distributions of points. The convergent rate is slower on a finer distribution of points.

The paper is organized as follows: in section 2, the numerical method is presented and some numerical tests are shown in section 3.

2. Numerical method

2.1. Least Squares approximation of a function and its derivatives

The least squares method can be applied to very irregular geometries. In many practical applications the mesh plays the most important role in determining the solution and many solvers loose their accuracy if the mesh is poorly constructed. An advantage of the least squares method is that it does not require grids to approximate the function and its derivatives.

Let $f(\vec{x})$ be a scalar function and f_i its values at $\vec{x}_i \in \Omega \subset R^d (d = 1, 2, 3)$ for $i = 1, 2, \ldots, N$, where N is the total number of points in Ω. We consider

the problem to approximate a function $f(\vec{x})$ and its derivatives at position $\vec{x}$ in terms of the values of its neighboring cloud of points. In order to restrict the number of points we associate a weight function $w = w(\vec{x}_i - \vec{x}; h)$ with small compact support, where h determines the size of the support. The constant h is similar to the smoothing length in the classical SPH method. The weight function can be quite arbitrary. In our computation, we consider a Gaussian weight function in the following form

$$w(\vec{x}_i - \vec{x}; h) = \begin{cases} exp(-\alpha \frac{\|\vec{x}_i - \vec{x}\|^2}{h^2}), & \text{if } \frac{\|\vec{x}_i - \vec{x}\|}{h} \leq 1 \\ 0, & \text{else,} \end{cases}$$

with α being a positive constant. The size of the support h defines a set of neighboring points around $\vec{x}$. Let $P(\vec{x}, h) = \{\vec{x}_i : i = 1, 2, \ldots, n\}$ be the set of n neighboring points of $\vec{x}$ in a ball of radius h. The radius h should be taken larger if a function has to be approximated by a higher degree of polynomials. For example, for a polynomial of second degree in $3D$, one needs at least 10 neighboring points such that h has to be chosen accordingly.

The approximation of a function and its derivatives can be computed easily and accurately by using the Taylor series expansion and the least squares approximation. We write a Taylor expansion around the point $\vec{x}$ with unknown coefficients and then compute these coefficients by minimizing a weighted error over the neighboring points.

Consider the Taylor expansion of $f(\vec{x}_i)$ around $\vec{x}$

$$\begin{aligned} f(\vec{x}_i) = f(\vec{x}) &+ \sum_{k=1}^{3} f_k(\vec{x})(x_{ki} - x_k) \\ &+ \frac{1}{2} \sum_{k,l=1}^{3} f_{kl}(\vec{x})(x_{ki} - x_k)(x_{li} - x_l) + e_i \,, \end{aligned}$$

for $i = 1, \ldots, n$, where e_i is the error in the Taylor expansion at the points $\vec{x}_i$. The symbols x_{1i}, x_{2i} and x_{3i} are denoted by the x, y and z components of the position $\vec{x}_i$, respectively. The unknowns f, f_k and $f_{kl} (= f_{lk})$ for $k, l = 1, 2, 3$ are computed by minimizing the error e_i for $i = 1, 2, \ldots, n$. The system of equations can be written as

$$\vec{e} = M\vec{a} - \vec{b}, \tag{2.1}$$

where $M =$

$$\begin{pmatrix} 1 & dx_1 & dy_1 & dz_1 & \frac{1}{2}dx_1^2 & dx_1dy_1 & dx_1dz_1 & \frac{1}{2}dy_1^2 & dy_1dz_1 & \frac{1}{2}dz_1^2 \\ 1 & dx_2 & dy_2 & dz_2 & \frac{1}{2}dx_2^2 & dx_2dy_2 & dx_2dz_2 & \frac{1}{2}dy_2^2 & dy_2dz_2 & \frac{1}{2}dz_2^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & dx_n & dy_n & dz_n & \frac{1}{2}dx_n^2 & dx_ndy_n & dx_ndz_n & \frac{1}{2}dy_n^2 & dy_ndz_n & \frac{1}{2}dz_n^2 \end{pmatrix},$$

$\vec{a} = [f, f_1, f_2, f_3, f_{11}, f_{12}, f_{13}, f_{22}, f_{23}, f_{33}]^T$,
$\vec{b} = [f_1, f_2, \ldots, f_n]^T$,

$\vec{e} = [e_1, e_2, \ldots, e_n]^T$.
The symbols dx_i, dy_i, dz_i denote $x_{i1} - x_1, x_{i2} - x_2, x_{i3} - x_3$, respectively, for $i = 1, 2, \ldots, n$.

For $n > 10$, this system is over-determined for the ten unknowns f, f_k and f_{kl} for $k, l = 1, 2, 3$.

The unknown vector $\vec{a}$ is obtained from a weighted least squares method by minimizing the quadratic form

$$J = \sum_{i=1}^{n} w_i e_i^2 \tag{2.2}$$

which can be expressed in the form

$$J = (M\vec{a} - \vec{b})^T W (M\vec{a} - \vec{b})$$

where

$$W = \begin{pmatrix} w_1 & 0 & \cdots & 0 \\ 0 & w_2 & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & w_n \end{pmatrix}.$$

The minimization of J formally yields

$$\vec{a} = (M^T W M)^{-1} (M^T W)\vec{b}. \tag{2.3}$$

The Taylor expansion may include higher order expansion and appropriate discrete weight functions can be used to force the least square approximations to recover finite difference discretization.

2.2. Least squares approach for the Poisson equation

In this approach we do not discretize the Poisson equation directly like in classical methods. We solve it by an iterative process where we enforce the Passion equation and boundary conditions to be satisfied in every iteration. Consider the following Poisson equation

$$\Delta u = f \quad \text{in} \quad \Omega \tag{2.4}$$

with Dirichlet boundary condition

$$u = g \quad \text{on} \quad \Gamma \tag{2.5}$$

or Neumann boundary condition

$$\frac{\partial u}{\partial \vec{n}} = g \quad \text{on} \quad \Gamma \tag{2.6}$$

or mixed boundary conditions.

In the previous section, we have presented the least squares method to approximate a function and its derivatives at an arbitrary point from the values of its neighboring points. In this case, the situation is slightly different since the values of u on the discrete points are not known a priori. This means that if the vector $\vec{b}$ in (2.3) is unknown, we cannot determine the coefficient vector $\vec{a}$. Therefore, we prescribe an initial guess $u^{(0)}$, of the value u at all points. Now we consider the problem of determining u at an arbitrary particle position $\vec{x}$ from its neighboring points $\vec{x}_i,\ i = 1, \ldots n$. As described in the previous section, we again consider a Taylor expansion of u at $\vec{x}$

$$u^{(\tau)}(\vec{x}_i) = u^{(\tau+1)}(\vec{x}) + \sum_{k=1}^{3} u_k^{(\tau+1)}(\vec{x})(x_{ki} - x_k) + \frac{1}{2}\sum_{k,l=1}^{3} u_{kl}^{(\tau+1)}(\vec{x})(x_{ki} - x_k)(x_{li} - x_l) + e_i^{(\tau+1)} \tag{2.7}$$

for $\tau = 0, 1, 2, \ldots$, where $u^{(0)}(\vec{x}_i)$ are known initial values. We apply the condition that the Poisson equation (2.4) must be satisfied at $\vec{x}$. For this, we have to add the following equation in the above n equations

$$f = u_{11}^{(\tau+1)}(\vec{x}) + u_{22}^{(\tau+1)}(\vec{x}) + u_{33}^{(\tau+1)}(\vec{x}). \tag{2.8}$$

For the Neumann boundary condition (2.6) we have to add the extra equation for the boundary point $\vec{x}$

$$g = u_1^{(\tau+1)}(\vec{x})n_x + u_2^{(\tau+1)}(\vec{x})n_y + u_3^{(\tau+1)}(\vec{x})n_z, \tag{2.9}$$

where n_x, n_y, n_z are the x, y, z components of the unit normal vector $\vec{n}$ on the boundary at $\vec{x}$. Hence we have a system of $n + 2$ equations with 10 unknowns and in general we have $n \geq 10$.

We obtain the coefficients

$$u^{(\tau+1)}, u_1^{(\tau+1)}, u_2^{(\tau+1)}, u_3^{(\tau+1)}, u_{11}^{(\tau+1)}, u_{12}^{(\tau+1)}, u_{13}^{(\tau+1)}, u_{22}^{(\tau+1)}, u_{23}^{(\tau+1)}, u_{33}^{(\tau+1)}$$

for $\tau = 1, 2, \ldots$ at $\vec{x}$ by minimizing

$$J = \sum_{i=1}^{n} w_i (e_i^{(\tau+1)})^2 + (\Delta u^{(\tau+1)} - f)^2 + (\frac{\partial u^{(\tau+1)}}{\partial \vec{n}} - g)^2. \tag{2.10}$$

Similarly, the minimization of J is given by

$$\vec{a}^{(\tau+1)} = (M^T W M)^{-1}(M^T W)\vec{b}^{(\tau)}, \tau = 0, 1, \ldots, \tag{2.11}$$

where the matrices and the vectors differ from (2.3) and are given by
$M =$

$$\begin{pmatrix} 1 & dx_1 & dy_1 & dz_1 & \frac{1}{2}dx_1^2 & dx_1dy_1 & dx_1dz_1 & \frac{1}{2}dy_1^2 & dy_1dz_1 & \frac{1}{2}dz_1^2 \\ 1 & dx_2 & dy_2 & dz_2 & \frac{1}{2}dx_2^2 & dx_2dy_2 & dx_2dz_2 & \frac{1}{2}dy_2^2 & dy_2dz_2 & \frac{1}{2}dz_2^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & dx_n & dy_n & dz_n & \frac{1}{2}dx_n^2 & dx_ndy_n & dx_ndz_n & \frac{1}{2}dy_n^2 & dy_ndz_n & \frac{1}{2}dz_n^2 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & n_x & n_y & n_z & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$W = \begin{pmatrix} w_1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & w_2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & w_n & 0 & 0 \\ 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 1 \end{pmatrix},$$

$\vec{a}^{(\tau+1)} = [u^{(\tau+1)}, u_1^{(\tau+1)}, u_2^{(\tau+1)}, u_3^{(\tau+1)}, u_{11}^{(\tau+1)}, u_{12}^{(\tau+1)}, u_{13}^{(\tau+1)}, u_{22}^{(\tau+1)}, u_{23}^{(\tau+1)}, u_{33}^{(\tau+1)}]^T$,
$\vec{b}^{(\tau)} = [u_1^{(\tau)}, u_2^{(\tau)}, \ldots, u_n^{(\tau)}, f, g]^T$.

Note that one can substitute the equation (2.8) into (2.7) such that the number of unknowns can be reduced. For example, from (2.8) we have

$$u_{33}^{(\tau+1)}(\vec{x}) = f - u_{11}^{(\tau+1)}(\vec{x}) - u_{22}^{(\tau+1)}(\vec{x}) \tag{2.12}$$

which can be substituted in (2.7) so that the number of unknowns reduces into 9 for interior points. Hence, instead of the 10×10 matrix one has to invert the 9×9 matrix. It does not reduce the computational costs much. In this case the coefficients of the matrix M and the vector b differ from above. But in both cases, the convergent rate remains the same.

The iterations are performed for all points. After each iteration, the new values $u^{(\tau+1)}$ are then assigned new function values. This is a local solution procedure. For each point, for example, in $3D$-case one has to invert a 10×10 matrix. This can be slower than other classical methods for Poisson equation, but in our case, there is no effort to generate the mesh and the solution can be obtained for arbitrary irregular geometry.

The iteration is stopped if the error satisfies

$$\frac{\sum_{i=1}^{N} |u_i^{\tau+1} - u_i^{(\tau)}|}{\sum_{i=1}^{N} |u_i^{(\tau+1)}|} < \epsilon \tag{2.13}$$

and the solution is defined by $u(x_i) := u^{(\tau+1)}(x_i)$ as τ tends to infinity. The parameter ϵ is a very small positive constant and can differ according to the

problems and value of h. One can take variable h according to the topology. We have considered constant h. The convergence rate is faster if h is taken larger. The value of h can be taken larger either by increasing the distance between points or by simply taking a larger factor for the same distance.

3. Numerical Tests

The numerical experiments are performed in the two dimensional space. We have computed the Poisson equation in a unit square, where the analytical solutions are available. The distributions of points are considered in regular as well as irregular structures. The regular points are generated with the space size $\Delta x = 0.04$. For the irregular case, the boundaries are replaced by regular points of spacing 0.04 and the distribution of interior points are considered quite non-uniform as shown in Fig.1. The size of support for the weight function for both types of distribution of points is considered as $h = 0.12$. As initial guess for $u^{(0)}$, we have chosen $u^{(0)}(\vec{x}_i) = 0$ at all points.

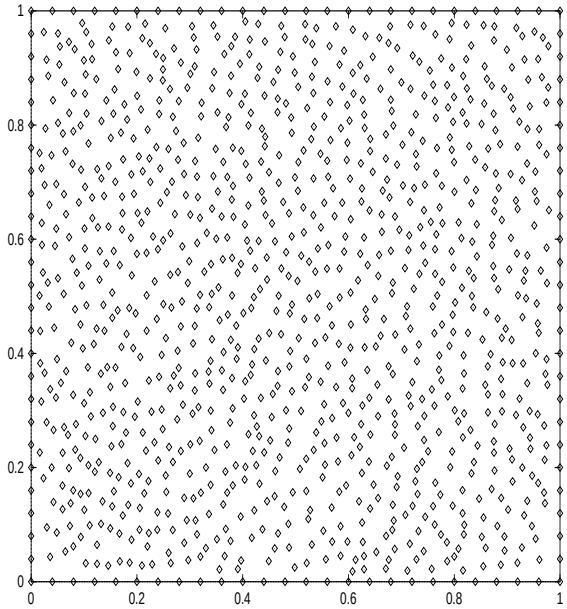


Fig. 1. *Non-uniform distribution of particles*

In the following we have considered the three problems: Dirichlet, Neumann and the mixed boundary value problems in a unit square.

3.1. Dirichlet boundary value problem

We consider the Dirichlet boundary value problem

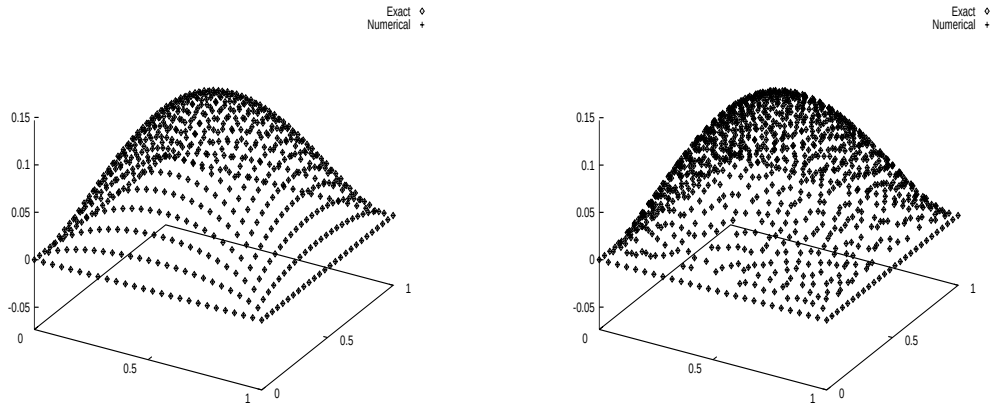
$$\Delta u = -2 \quad \text{in} \quad (0,1) \times (0,1)$$

$$u = 0 \quad \text{on} \quad x = 0,\ y = 0,\ x = 1 \text{ and } y = 1.$$

The analytical solution of this problem is given by

$$u(x,y) = (1-x)x - \frac{8}{\pi^3}\sum_{n=1}^{\infty}\left[\frac{\sinh[(2n-1)\pi(1-y)] + \sinh[(2n-1)\pi y]}{\sinh(2n-1)\pi}\right]\cdot\frac{\sin(2n-1)\pi x}{(2n-1)^3}.$$

In Fig. 2, we have compared the exact solutions with the numerical ones. The figures show good agreements between the exact and numerical solutions for regular as well as irregular distribution of points.



Regular points *Irregular points*

Fig. 2. *Comparison between the exact and numerical solutions for the Dirichlet problem*

3.2. Neumann boundary value problem

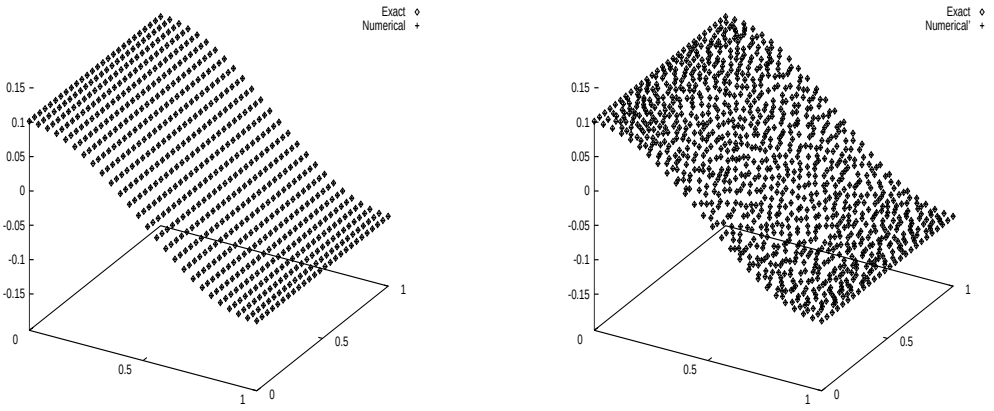
Next, we consider the Neumann boundary value problem:

$$\Delta u = -cos\pi x \quad \text{in} \quad (0,1)\times(0,1)$$
$$\frac{\partial u}{\partial \vec{n}} = 0 \text{ on } x = 0,\ y = 0,\ x = 1 \text{ and } y = 1.$$

The analytical solution of this problem is given by

$$u(x,y) = \frac{1}{\pi^2}\cos\pi x.$$

In Fig.3 we have plotted the numerical solutions against the analytical ones for both types of distributions of points. We see that the numerical solutions matched perfectly with the analytical solutions.



Regular points *Irregular points*

Fig. 3. *Comparison between the exact and numerical solutions for the Neumann problem*

3.3. Mixed boundary value problem

Finally, we consider the mixed boundary value problem

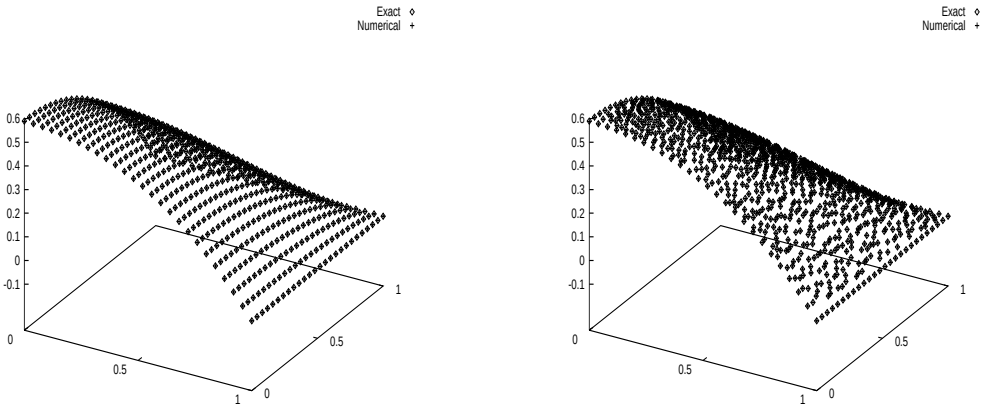
$$\begin{aligned} &\Delta u = -2 \quad \text{in} \quad (0,1)\times(0,1) \\ &u = 0 \quad \text{on} \quad x = 1 \quad \text{and} \quad y = 1 \\ &\frac{\partial u}{\partial \vec{n}} = 0 \quad \text{on} \quad x = 0 \quad \text{and} \quad y = 0. \end{aligned}$$

The analytical solution of this problem is given by

$$u(x,y) = (1-y)^2 + \frac{32}{\pi^3}\sum_{n=0}^{\infty} \frac{(-1)^{n+1}\cos[(2n+1)\pi\frac{y}{2}]\cosh[(2n+1)\pi\frac{x}{2}]}{(2n+1)^3\cosh(2n+1)\frac{\pi}{2}}.$$

The numerical solutions are plotted against the analytical solutions in Fig.4. For both types of distributions of points the analytical solutions are identical with the numerical ones.

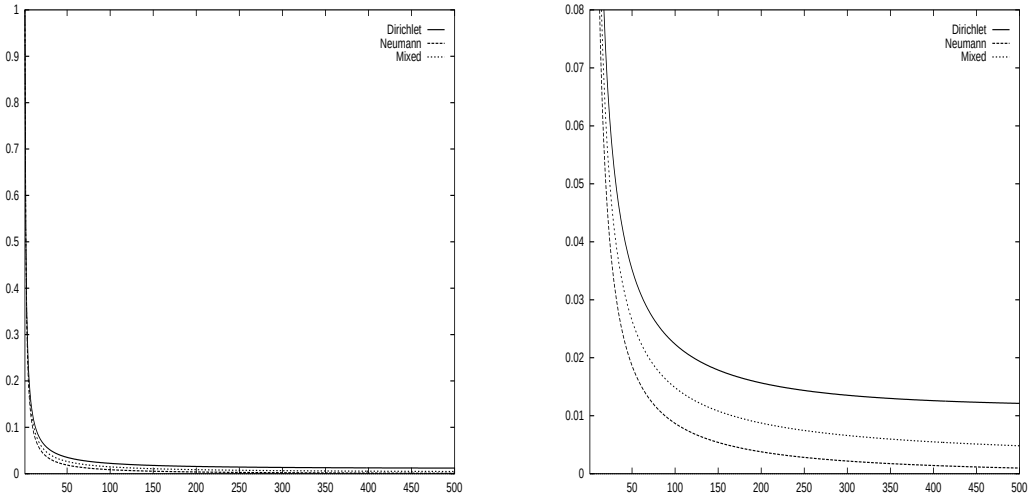
In Fig. 5 the errors defined in (2.13) for all three boundary value problems are plotted in every iterations. In all cases the errors are decaying exponentially and converge asymptotically to some small positive constants. It can be



Regular points *Irregular points*

Fig. 4. *Comparison between the exact and numerical solutions for mixed boundary value problem*

also seen that there is no oscillation and the scheme is stable. The tuning parameters for truncating iterations depend on the problems. If we look closely at the errors plotted in Fig. 5(b), we see that the asymptotic value for the Dirichlet problem is larger than that for the other two problems. It is smallest for the Neumann boundary value problem.



(a) (b)

Fig. 5. *Errors versus iterations for three boundary value problems*

4. Conclusion

A numerical model for solving the Poisson equation in grid free structure is presented. The computational domain is approximated by a finite number of points. In each point the solution is approximated. The distribution of points is not required to be regular. The method is based on the weighted least squares method where the Poisson equation and boundary conditions are enforced to to be satisfied in every iterations. This is a local iterative process. The purpose of developing this Poisson solver is to simulate incompressible flows by the Lagrangian particle method. In this case the particles are themselves grid points and can be distributed quite irregularly during the flow simulation, like in Fig. 1. The method can also be applied for any elliptic boundary value problem and is especially appropriate for complicated geometry, where the mesh generation is very poor. However, no comparison study has been done, yet.

The convergence rate depends on the size of the support of weight function. It is faster for larger h and slower for smaller h. Therefore, the multigrid method could be quite appropriate in order to decrease the number of iterations. We are looking forward to including the multigrid method in order to accelerate the computation. Furthermore, the main goal of our future work is to apply this method to incompressible flow problems.

Acknowledgment: The first author thanks Deutsche Forschungsgemeinschaft for the financial support.

References

[1] T. Belytschko, Y. Krongauz, D. Organ, M. Flemming, P. Krysl *Meshless methods: An overview and recent developments*; Comput. Methods Appl. Mech. Engrg. **139** (1996) 3- 47

[2] A. Chorin, *Numerical solution of the Navier-Stokes equations*; J. Math. Comput. **22** (1968) 745-762

[3] G.A Dilts, *Moving least squares particle hydrodynamics I, consistency and stability*; Hydrodynamics methods group report, Los Alamos National Laboratory, 1996

[4] S.M. Deshpande and P.S. Kulkarni, *New developments in kinetics schemes*; Comp. Math. Appl., **35**, (1998) 75-93

[5] R. A. Gingold and J. J. Monaghan, *Smoothed particle hydrodynamics: theory and application to non-spherical stars*; Mon. Not. Roy. Astron. Soc. **181**,(1977) 375-389

[6] J. Kuhnert, *General smoothed particle hydrodynamics*; Ph.D. thesis, Kaiserslautern University, Germany, 1999

[7] L. B. Lucy, *A numerical approach to the testing of the fission hypothesis*; Astron. J., **82**, (1977) 1013

[8] J.J.Monaghan, *Smoothed particle hydrodynamics*; Annu. Rev. Astron. Astrop, **30**,(1992) 543-574

[9] J.J.Monaghan, *Simulating free surface flows with SPH*; J. Comput. Phys., **110**, (1994) 399

[10] J. J. Monaghan, A. Kocharyan, *SPH simulation of multi-phase flow*; Computer Phys. Commun., **87**, (1995) 225-235

[11] J.P.Morris, P.J.Fox and Y.Zhu, *Modeling Low Reynolds Number Incompressible Flows Using SPH*; J. Comput. Phys., **136**,(1997) 214-226

[12] S. Tiwari, *A least squares SPH approach for compressible flows*, preprint ITWM, Kaiserslautern Germany, 2000 (to appear in Proceedings of the 8th International Conference on Hyperbolic Problems Hyp2000)

[13] S. Tiwari, J. Kuhnert, *LSQ-SPH method for simulations of free surface flows*, preprint ITWM, Kaiserslautern, Germany, 2000

[14] S. Tiwari and S. Manservisi *Modeling incompressible Navier-Stokes flows by LSQ-SPH*, preprint ITWM, Kaiserslautern, Germany, 2000

Bisher erschienene Berichte des Fraunhofer ITWM

Die PDF-Files der folgenden Berichte finden Sie unter:
www.itwm.fhg.de/zentral/berichte.html

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

A Finite - Volume Particle Method for Compressible Flows

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

2. M. Feldmann, S. Seibold

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

In this paper, a combined approach to damage diagnosis of rotors is proposed. The intention is to employ 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 S., 1998)

3. Y. Ben-Haim, S. Seibold

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

Damage diagnosis based on a bank of Kalman filters, each one conditioned on a specific hypothesized system condition, is a well recognized and powerful diagnostic tool. This multi-hypothesis approach can be applied to a wide range of damage conditions. In this paper, we will focus on the diagnosis of cracks in rotating machinery. The question we address is: how to optimize the 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 S., 1998)

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

Three-dimensional Radiative Heat Transfer in Glass Cooling Processes

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

5. A. Klar, R. Wegener

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

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

Part II: Numerical and stochastic investigations

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

6. A. Klar, N. Siedow

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

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

7. I. Choquet

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

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

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

Efficient Texture Analysis of Binary Images

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

9. J. Orlik

Homogenization for viscoelasticity of the integral type with aging and shrinkage

A multi-phase composite with periodic distributed inclusions with a smooth boundary is considered in this contribution. The composite component materials are supposed to be linear viscoelastic and aging (of the non-convolution integral type, for which the Laplace transform with respect to time is not effectively applicable) and are subjected to isotropic shrinkage. The free shrinkage deformation can be considered as a fictitious temperature deformation in the behavior law. The procedure presented in this paper proposes a way to determine average (effective homogenized) viscoelastic and shrinkage (temperature) composite properties and the homogenized stress-field from known properties of the

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

10. J. Mohring

Helmholtz Resonators with Large Aperture

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

11. H. W. Hamacher, A. Schöbel

On Center Cycles in Grid Graphs

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

12. H. W. Hamacher, K.-H. Küfer

Inverse radiation therapy planning - a multiple objective optimisation approach

For some decades radiation therapy has been proved successful in cancer treatment. It is the major task of clinical radiation treatment planning to realize on the one hand a high level dose of radiation in the cancer tissue in order to obtain maximum tumor control. On the other hand it is obvious that it is absolutely necessary to keep in the tissue outside the tumor, particularly in organs at risk, the unavoidable radiation as low as possible.
No doubt, these two objectives of treatment planning - high level dose in the tumor, low radiation outside the tumor - have a basically contradictory nature. Therefore, it is no surprise that inverse mathematical models with dose distribution bounds tend to be infeasible in most cases. Thus, there is need for approximations compromising between overdosing the organs at risk and underdosing the target volume.
Differing from the currently used time consuming iterative approach, which measures deviation from an ideal (non-achievable) treatment plan using recursively 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 S., 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 S., 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 S., 1999)

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

A new discrete velocity method for Navier-Stokes equations

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

16. H. Neunzert

Mathematics as a Key to Key Technologies

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

17. J. Ohser, K. Sandau

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

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

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

Solving nonconvex planar location problems by finite dominating sets

It is well-known that some of the classical location problems with polyhedral gauges can be solved in polynomial time by finding a finite dominating set, i. e. a finite set of candidates guaranteed to contain at least one optimal location.
In this paper it is first established that this result holds for a much larger class of problems than currently considered in the literature. The model for which this result can be proven includes, for instance, location problems with attraction and repulsion, and location-allocation problems. Next, it is shown that the approximation of general gauges by polyhedral ones in the objective function of our general model can be analyzed with regard to the subsequent error in the optimal objective value. For the approximation problem two different approaches are described, the sandwich procedure and the greedy algorithm. Both of these approaches lead - for fixed epsilon - to polynomial approximation algorithms with accuracy epsilon for solving the general model considered in this paper.
Keywords:
Continuous Location, Polyhedral Gauges, Finite Dominating Sets, Approximation, Sandwich Algorithm, Greedy Algorithm
(19 S., 2000)

19. A. Becker

A Review on Image Distortion Measures

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

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

Polyhedral Properties of the Uncapacit*ated 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 S., 2000)

21. H. W. Hamacher, A. Schöbel

Design of Zone Tariff Systems in Public Transportation

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

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

The Finite-Volume-Particle Method for Conservation Laws

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

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

Location Software and Interface with GIS and Supply Chain Management

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

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

Mathematical Modelling of Evacuation Problems: A State of Art

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

25. J. Kuhnert, S. Tiwari

Grid free method for solving the Poisson equation

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

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